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Review of Potential Models for UF_6 Dispersion

R. I. Sykes
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ARAP Group
California Research and Technology Division
The Titan Corporation

July 1992

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LOCKHEED MARTIN ENERGY SYSTEMS, INC.
FOR THE UNITED STATES
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GASEOUS DIFFUSION PLANT
SAFETY ANALYSIS REPORT UPGRADE PROGRAM

REVIEW OF POTENTIAL MODELS FOR UF_6 DISPERSION

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EXECUTIVE SUMMARY

A survey of existing atmospheric dispersion models has been conducted to determine the most appropriate basis for the development of a model for predicting the consequences of an accidental UF_6 release. The model is required for safety analysis studies and should therefore be computationally efficient. The release of UF_6 involves a number of physical phenomena which make the situation more complicated than passive dispersion of a trace gas. The safety analysis must consider the density variations in the UF_6 cloud, which can be heavier or lighter than the ambient air. The release also involves rapid chemical reactions and associated heat release, which must be modeled. Other Department of Energy storage facilities require a dense gas prediction capability, so the model must be sufficiently general for use with a variety of release scenarios.

The special problems associated with UF_6 make it unique, so there are very few models with existing capability for the problem. There are, however, a large number of dense gas dispersion models, some with relevant chemical reaction modeling, that could potentially form the basis of an advanced UF_6 model. We have examined a large selection of possible candidates, and selected 5 models for detailed consideration. These comprise:

1. PLM89A — Martin Marietta Energy Systems, Inc., UF_6 model
2. TRIAD — NOAA UF_6 model
3. HGSYSTEM — Industry consortium dense gas model
4. ADAM — Air Force dense gas model
5. SLAB — Lawrence Livermore National Laboratory dense gas model

The first two candidates were specifically developed for UF_6 dispersion prediction, while the remaining three are for general dense gas releases. HGSYSTEM and ADAM include models for hydrogen fluoride chemistry, one of the products of UF_6 reaction with water.

None of the candidates completely meet all the requirements of the safety analysis model and we detail the necessary development for each of the individual models. TRIAD is designed principally for the emergency response application, with its emphasis on a general wind field description and Gaussian puff framework. The dynamic effects of the dense gas release and the

reactive chemistry are modeled very crudely as part of the source specification. These effects are an important aspect for safety analysis studies, while the precise trajectory of the release is only required for an actual accident response. The other four models all contain a more detailed description of the dynamics, and are therefore considered more suitable for the current application unless a requirement for emergency response application is added to the requirement for safety analysis.

The safety analysis model could be developed from any of the other four models with a reasonable level of effort. There are several aspects of the problem that require modification to any of the models, while some features are already present in some of the models. For example, PLM89A already contains a sophisticated treatment of the UF_6 chemistry, while SLAB contains no chemistry. However, PLM89A's treatment of dense gas effects and transient dynamic processes is inferior to SLAB's. Specific model development requirements are briefly as follows:

PLM89A	-	extend transient source model to describe nonlinear chemistry and dynamics
	-	account for suppression of vertical mixing in dense ground-hovering cloud
HGSYSTEM	-	extend reaction scheme to include UF_6 chemistry
ADAM	-	extend reaction scheme to include UF_6 chemistry
SLAB	-	implement reactive chemistry for UF_6

Among these four models, HGSYSTEM and SLAB have undergone the most extensive comparison with atmospheric release data from dense gas experiments (the dense gas dispersion module within HGSYSTEM is actually the HEGADAS model which has been used in many model evaluation studies). ADAM has been compared with a number of experimental measurements, but not as extensively as HEGADAS and SLAB. PLM89A has not been compared with the same range of data, and therefore cannot claim the same validation support as the other models. Two points need to be made with regard to existing model evaluation, however. First, the results quoted in the literature are generally based on subsets of the observational data. These subsets are apparently designed to provide a comparison to the maximum centerline plume concentration, since any non-monotonically decreasing concentrations are ignored, but there is no guarantee that the sampler network actually measured the maximum value. The discrepancy between the model predictions and the selected observations should therefore be augmented by an estimate of the variability in the sampling procedure as well as the natural uncertainty inherent in the atmospheric dispersion process

to give a realistic estimate of model reliability. Second, the addition of the complicating physical effects of exothermic chemistry is almost certain to decrease the accuracy of the model below that of the non-reacting dense gas situation.

The features requiring improved treatment for all models are:

1. turbulent atmospheric dispersion
2. building and terrain effects
3. turbulent chemical reaction and exothermic heat release

Atmospheric dispersion is currently based on empirical Pasquill-Gifford-Turner (PGT) stability classification. SLAB uses a more general turbulence-based scheme, and we recommend that this approach be extended to a full description of boundary layer diffusion using estimated profiles of velocity and turbulence. Current knowledge of the structure of the planetary boundary layer is sufficiently well developed to allow such a scheme to be implemented, and we propose specific recommendations for the dispersion modeling. This improvement would give the safety analysis model a sounder physical basis and extend its range of applicability to more general release and atmospheric conditions.

The presence of very large buildings in the vicinity of potential accidental releases can have significant influence on the dispersion, especially for dense clouds. We recommend a simple limiting of the lateral dispersion to account for the building 'canyon' effects, and an increase in the surface roughness estimate if the model is employing such information to determine the ambient turbulence levels.

The turbulent chemical reaction process is probably the most complicated phenomenon involved in the UF_6 release. PLM89A uses a turbulence-based reaction timescale to account for the finite mixing rate, while the other models (HGSYSTEM and ADAM) use steady-state chemistry assuming instantaneous reaction. The present state of understanding of turbulent reactive chemistry makes its parameterization uncertain, and we believe that use of 'instantaneous' plume spread estimates in conjunction with instantaneous chemistry is currently as reliable as the turbulent mixing

estimates. The proposed atmospheric dispersion model framework is designed to give the capability for predicting instantaneous or time-average plume spreads.

The reaction between UF_6 and water is strongly exothermic and can switch the cloud buoyancy from negative to positive. The details of the heat release are uncertain, however, since the details of the turbulent mixing are uncertain. If the heat is released at the edges of the dense, ground-hovering cloud, then it may be possible for a buoyant cloud of reaction products to effectively separate from the underlying dense plume. We discuss a two-plume approach for modeling this phenomenon, with the heated reaction products being transferred from the initial dense UF_6 plume into an upper buoyant plume. This simplified modeling relies on its own internal set of assumptions about the interfacial transport of the various species, and we recommend that some form of detailed study be made to determine the nature and extent of the non-uniform heating effects. Any implementation of the two-plume model will require significant model development and this should only be undertaken with some guidance from more reliable investigations. High-resolution, three-dimensional, dynamic models could be used to provide information for the development of simplified representations.

The incorporation of the appropriate chemistry and dispersion representations into one of the candidate models will provide a reasonably complete description of UF_6 dispersion for use in the safety analysis. The level of uncertainty in the predictions of the final model should not be underestimated, however. While the principal physical processes will be represented in the best available manner within the context of a simplified model, the uncertainties in the predictions are likely to be larger than the currently reported discrepancies between dense gas measurements and predictions. Whichever route to a safety analysis model is chosen, it would be very desirable to perform an extensive model evaluation study for the final model as a means of quantifying the uncertainty in the results. We would expect the model to correctly estimate the results of anticipated scenarios to within an order of magnitude. Any significant reduction in this order of magnitude uncertainty would need to be established by careful comparisons between field tests and model simulations.

CONTENTS

1. INTRODUCTION

The use and storage of UF_6 in Department of Energy (DOE) facilities poses a potential hazard in the event of an accidental release. In order to assess the risk and possible effect on local populations, a prediction of the evolution of the material concentrations and composition in the atmosphere is required. The behavior of UF_6 is more complex than most materials, since it involves an exothermic chemical reaction with water and the production of secondary species such as hydrogen fluoride (HF), which are themselves hazardous and reactive. The release also involves a phase change, since UF_6 is not typically stored at atmospheric pressure, with associated source momentum and buoyancy effects. UF_6 gas is much denser than air, so the possibility exists for the gas cloud to remain confined close to the ground as a stable blanket, but the heat generated by the reactive chemistry can switch the sign of the relative buoyancy of the cloud and cause it to rise. The polymerization of HF can also produce denser-than-air clouds, restricting the vertical mixing of the hazardous material. The initial momentum of the release can also project the material upward into the atmosphere before it falls to the surface as a dense cloud. These dynamical and chemical phenomena all occur within the turbulent atmosphere in the presence of buildings and terrain; therefore require a relatively sophisticated model to account for all the effects.

Martin Marietta Energy Systems, Inc. (Energy Systems) has developed a dispersion model, PLM89A, to account for the major features of an atmospheric release of UF_6 (Bloom et al., 1989). In an earlier review of the Energy Systems model (Hicks et al., 1985), several shortcomings in the existing version of PLM89A were noted, most important being the inadequate treatment of transient releases, the neglect of proper thermodynamic exchanges in situations with pre-existing water droplets (i.e., fog), and the neglect of any concentration fluctuations. Since that time, other models have been developed to predict various types of release, and the objective of the current review is to determine the most appropriate basis for the implementation of an acceptable model for a safety analysis of possible accidental UF_6 releases. The generality of the final safety analysis model will also make it suitable for the prediction of the effects of accidental releases of other dense gases without the complicating effects of UF_6 chemistry.

The definition of acceptability obviously depends on the context of the model application. In this case, the model is required for safety analysis studies so detailed predictions are not necessary. We can never know the details of the situation for an anticipated accidental release, and the true

"worst case" is impossible to define since the release and meteorological conditions can vary so widely. The model must therefore provide a reasonable representation of the major physical and chemical phenomena, consistent with the level of accuracy of the input data and the range of uncertainty of the flow field. The flow field uncertainty does not include all possible flow conditions, since we can consider subsets of the meteorology (e.g., low-wind speed and stable atmosphere). This is the standard method for safety assessment, and the model accuracy requirement is defined in terms of the general range of flow variation within the class of conditions to be assessed. Obviously, a detailed model may meet and perhaps exceed this accuracy requirement, but the disadvantage of a complex model lies in the difficulty of providing the input information and the resources needed to obtain a prediction. We shall discuss the practical implementation of various modeling techniques in the next section. The requirements for a safety analysis model are quite different than those of an emergency response model. One wants an emergency response model to incorporate as many of the particular details of the moment as are deemed important enough to justify the added time and expense they involve. One wants it to "nowcast" the probabilities of hazardous concentrations reaching vulnerable populations. A good emergency response model could provide the basis for a very comprehensive safety analysis. The process would involve estimating the possible release scenarios in combination with possible meteorological scenarios, and running the emergency response for a sufficiently large number of the possible combinations to obtain good statistics on the resultant probability of significant injuries. However, the safety analysis does not necessarily share the prerequisite to incorporate all the details of a large number of particular scenarios. It only needs to provide reasonably accurate estimates for any likely conditions which may lead to significant injuries. Risk assessment will also require estimates of the probabilities associated with these serious consequence scenarios.

The specific locations for the application of the UF_6 safety analysis are the DOE plants in Portsmouth, Ohio and Paducah, Kentucky. It is desirable that the model have sufficient generality for it to be used for assessing other hazardous chemical release scenarios on other sites, but the principal application is UF_6 and the two named plants are the priority locations. Both sites have very large buildings in the vicinity of potential releases, and we must consider the effect of these buildings on the dispersion of the gas. It is also possible that the release will occur inside one of the buildings, so the external atmospheric source will be through doors, windows, containment breaches, or roof vents. We shall not consider the internal building flows in this review, but we recognize the possible source configurations and flow modifications induced by the building release.

The terrain around the Portsmouth and Paducah plants is not extreme. Paducah is relatively flat, with no hills in the immediate vicinity of the plant as large as some of the individual buildings. The Portsmouth plant is surrounded by gently rolling hills with 100- to 200-ft changes in elevation. It is not anticipated that strong flow modifications due to terrain will be experienced at either site, so extensive effort for terrain modeling should not be required. The large buildings located at the sites are more significant than the local terrain, and can clearly modify plume behavior in their immediate vicinity. The safety analysis model should therefore include some account of the building effects. We expect that the local meteorological monitoring will be sufficient to characterize the climatology around the plant, and that the assumption of homogeneous conditions will be reasonable. It is possible that there might be some shallow valley channelling involved in a dense gas release under light wind, stable meteorological conditions. This should be examined in relation to the statistical distribution of meteorological conditions.

2. REVIEW OF AVAILABLE MODELS

2.1 General Features of a Large Number of Models

The first candidate model for the prediction of a UF_6 release is obviously PLM89A, since it was specifically designed for the task. There are, however, several deficiencies in the model so the purpose of this review is to examine other candidates to determine the route to the development of the best model. To the best of our knowledge, only one other model has been specifically designed for the UF_6 prediction application, namely the TRIAD model of Hicks et al., 1989. There are, however, a large number of alternative atmospheric dispersion models that could form the basis of a UF_6 model. Since PLM89A presently does not meet all the requirements for the safety analysis model, some model development is inevitable and the extension of an existing dispersion model may be the most attractive course.

The complexity of the safety analysis requirement demands a number of features from the dispersion model, so we make a preliminary examination of a number of models to determine the list of capabilities of each. The list of models considered in this survey is presented in Table 2.1, with a brief description of each model. The list is far from exhaustive, since many atmospheric dispersion models are designed for very different applications from UF_6 release and would clearly require extensive modification for use as the safety analysis model. One of the key features of the UF_6 dispersion is the dense gas dispersion phenomena, so the bulk of Table 2.1 is composed of dense gas models which already contain a description of these effects. The surveys by Hanna (1987) and Hanna and Chang (1991) provided a very useful catalog of the dense gas models, as well as some evaluation data, and this information has been incorporated into this review.

The models may be divided into several broad categories according to their representation of the spatial structure of the gas cloud. Most of the models utilize shape assumptions, either Gaussian or box distributions, to reduce the computational load, and this can be implemented as a steady-state plume or as a transient puff. A more detailed approach involves solving the partial differential equations describing the full spatial dependence of the flow and concentration fields, an example being FEM3A, and the price of this increased generality is computational expense.

Table 2.2 contains a brief assessment of the various model capabilities of relevance to the safety analysis application. The specific features covered in this initial survey are as follows:

1. Ability to deal with transient releases (TR),
2. Representation of buoyant dynamics (DYN),
3. Representation of transient dynamics (TD),
4. Representation of turbulent dispersion (TURB),
5. Description of building effects (BLD),
6. Description of terrain effects (TER),
7. Description of UF_6 chemistry (UF_6).
8. Real-time data (emergency response application) (RLTM),
9. Representation of statistical fluctuations (FLUC),
10. Status of model evaluation (VAL), and
11. Separate modules for source representations and dispersion.

Table 2.1. List of models considered in initial screening

Model	Type	Reference	Status
PLM89A	Plume	Bloom et al., 1989	A
TRIAD	Puff	Hicks et al., 1989	A
D2DC	Plume	Whitacre et al. 1986	A
EAHAP	Plume	EAI, Concord, MA	
Eidswik		Eidswik, 1980	
EPIDIS	Plume	FSE, Sparta, NJ	
FEM3A	3D	Chan, 1988	A
HASTE		Paine et al., 1986	
AVACTA II	Plume	Zanetti et al., 1986	P
CARE	Plume	Verholek, 1986	P
CHARM	Plume	Elgroth & Smith, 1983	P
COBRA III	Plume	Alp 1985; Olivario et al., 1986	A
CRUNCH	Plume	Jagger, 1983	P
DEGADIS	Plume/puff	Havens & Spicer, 1985	A
DENZ	Puff	Fryer & Kaiser, 1979	P
HEAVYPUFF	Puff	Riso, Denmark	
HEGADAS	Plume	Colenbrander, 1980	A
INPUFF 2.0	Puff	Petersen & Lavdas, 1986	A
MIDAS	Plume	Pickard, Lowe & Garrick, DC	P
ModSys	Plume	Alp, 1985; Olivario et al., 1986	
PLUMEPATH	Plume	Ooms, 1972; Ooms et al., 1974	
RIMPUFF	Puff	Riso, Denmark	
SAFEMODS		Raj, 1981, 1985	
SAFER/TRACE		Safer, Westlake Village, CA	P
SLAB	Plume/puff	Ermak, 1990	A
SPILLS	Plume	Fleischer, 1980	
SRI PUFF	Puff	SRI International	
TRAUMA		Wheatley et al., 1985	
VAPID	Plume	Jemsen, 1983	
SAFE	Plume	AOSTRA, Edmonton, Alberta	P
SAFETI		Ale & Whitehouse, 1986	
TECJET	Plume	Ale & Whitehouse, 1986	
WHAZAN		Kayes, 1985	
MESOI	Puff	Ramsdell et al., 1983	A
SCIPUFF	Puff	Sykes et al., 1988	A
ADAM	Plume/puff	Raj and Morris, 1987	A
HGSYSTEM	Plume/puff	Witlox et al., 1990	A

A = available P = propietary

Table 2.2. Attributes of models considered in initial screening

Model	TR	DYN	TD	TURB	BLD	TER	UF_6	RLTM	FLUC	VAL	SRC
PLM89A	Y	Y	N	PG	N	N	Y	N	N	D	N
TRIAD	Y	B	N	PG/T	N	N	Y	Y	N	N	N
D2DC	Y	B	N		N	N	N	N	N	N	Y
EAHAP	Y	Y	D		N	N	N	N	N	D	Y
Eidswik	Y	D	D		N	N	N	N	N	D	N
EPIDIS	Y	D	D		N	N	N	N	Y	D	Y
FEM3A	Y	D	D	T	Y	Y	N	N	N	Y	N
HASTE	Y	Y	N		Y	N	N	Y	N	N	Y
AVACTA II	Y	B	N		N	Y	C	N	N	D	N
CARE	Y	D	D		Y	Y	C	Y	N	D	Y
CHARM	Y	Y	D		Y	N	C	Y	N	Y	Y
COBRA III	Y	D	D		N	N	N	N	N	D	Y
CRUNCH	C	D	N		N	N	N	N	N	D	N
DEGADIS	Y	D	D	PG	N	N	N	N	N	Y	Y
DENZ	I	D	D		N	N	N	N	N	D	N
HEAVYPUFF	I	Y	D		N	N	N	N	N	N	N
HEGADAS	Y	D	D	T	N	N	N	N	Y	Y	Y
INPUFF 2.0	Y	B	N	PG	N	N	N	N	N	Y	N
MIDAS	Y	Y	D		Y	Y	N	Y	N	D	Y
ModSys	Y	Y	D		N	N	C	N	Y	D	Y
PLUMEPATH	C	Y	N		N	N	N	N	N	N	N
RIMPUFF	Y	B	N		N	Y	N	Y	Y	D	Y
SAFEMODS	Y	Y	D		N	Y	C	Y	Y	D	Y
SAFER/TRACE	Y	D	D		N	Y	C	Y	N	Y	Y
SLAB	Y	Y	D	T	N	N	N	N	Y	Y	Y
SPILLS	Y	B	N		N	N	N	N	N	D	Y
SRI PUFF	Y	B	N		N	Y	N	N	N	D	N
TRAUMA	C	N	N		N	N	C	N	N	N	N
VAPID	Y	D	D		N	N	N	N	N	N	Y
SAFE	Y	B	N		N	N	C	Y	Y	N	N
SAFETI	Y	Y	D		N	N	N	N	N	D	Y
TECJET	C	Y	D		N	N	N	N	N	D	Y
WHAZAN	Y	Y	D		N	N	N	N	N	N	Y
MESOI	Y	B	N	PG	N	N	N	Y	N	Y	N
SCIPUFF	Y	B	B	T	N	N	N	Y	Y	D	N
ADAM	Y	Y	D	PG/T	N	N	C	N	N	D	Y
HGSYSTEM	Y	Y	D	PG/T	N	N	C	N	Y	D	Y

A brief comment on each of these features, including a key to the model capability nomenclature used in Table 2.2 and the perceived relative importance of the features, follow.

1. Ability to deal with transient releases (TR)

Each model is given one of three letters: Y if it models both continuous plumes and instantaneous releases, C if it models only continuous plumes, and I if it models only instantaneous releases. We consider it important that the Safety Analysis Model at least be able to deal with both continuous and instantaneous releases. Ideally, the model should be able to follow any transient evolution of the source.

2. Ability to deal with buoyant dynamics (DYN)

Each model is given one of four letters: Y if it models both dense and positively buoyant releases, N if it models only neutrally buoyant plumes, D is it models only dense releases, and B if it models only positively buoyant releases. We consider it essential that the Safety Analysis Model be able to deal with both aspects of buoyant dynamics, since they can contribute very significantly to the dispersion process.

3. Representation of transient dynamics (TD)

The ability to simulation the transient dynamics is considered separately, because many models make no distinction between the dynamics of a steady state plume and that of an instantaneous puff. We have made a distinction between 4 types of representation here: Y if the dynamics of plumes and puffs are dealt with differently for both positive and negative buoyancy, N if they are not, B if only for positive buoyancy, and D if only for negative buoyancy. This feature is not quite as important as (1) and (2), but the difference between the buoyant rise of a steady-state plume and a puff can be as much as a factor of 2.

4. Representation of turbulent dispersion (TURB)

This is perhaps the most important single feature of these models. We have tried to indicate whether the dispersion is based on simple Pasquill-Gifford correlations (denoted by PG) or on either

specified wind fluctuations or theoretical estimates of turbulence parameters (T). Some models contain options for the use of on-site wind fluctuation data, usually for the horizontal dispersion estimate, and these models are denoted as PG/T.

5. Description of building effects (BLD)

This feature is described by a simple Y or N depending upon whether the model attempts to include it or not. Considering the fact that some of the buildings involved contain up to 10^8 ft^3, this may be important for this particular safety analysis model. It can lead to close-in hot spots in the separated wake, and still be of some importance far downstream through its effect on equivalent source size. We should emphasize that treatment of building effects is usually very crude in the simple models.

6. Description of terrain effects (TER)

The incorporation of at least some effects of topography are indicated by a Y; the absence of any effects by an N. This should not be as important an issue as the buildings effect, since neither Portsmouth nor Paducah has major topographical features in the neighborhood of the plants.

7. Description of UF_6 chemistry (UF_6)

Only PLM89A and TRIAD have a Y for this feature to denote their attempt to include UF_6 chemistry. The C indicates that the model does include some other chemistry. An N indicates no inclusion of any chemistry.

8. Ability to use real-time data (emergency response application) (RLTM)

It seems extremely important for the facilities under consideration to have a model to guide decision makers during any real emergencies. For such an emergency response application it is essential to have some means of providing real-time meteorological data to the dispersion model. We have included this feature with a simple Y or N. We note, however, that the emergency response application can be substantially different from the safety analysis application, and that the latter is the principal focus of the present review.

9. Representation of statistical fluctuations (FLUC)

When modeling the spread of very toxic or highly reactive substances such as UF_6 and HF, we believe it is important to recognize the difference between the expected mean concentration distribution and that expected to occur over a short interval of time. The mean concentration may be expected to be reasonably smooth, but that occurring for any particular short instance of time may be expected to be much more random in character. Chemical reaction rates will be determined by local near-instantaneous concentration levels, and a short-time-interval exposure can induce chronic injuries for some toxic materials. This column indicates with a Y or an N whether the model does or does not make the distinction between different sample averaging times.

10. Status of model evaluation (VAL)

Model evaluation is an essential model feature, but hardly one which can be characterized by a few categories. It will be discussed in much more detail in Section 2.2. We only make very cursory distinctions in this column. We indicate with a Y if we know that the model has been the subject of evaluation by some independent party (i.e., someone other than the model developer). If we only know of evaluations done by the developer, this is indicated by a D. If even this is not available it is given an N.

11. Separate modules for source representations and dispersion (SRC)

The safety analysis model must consider a range of possible release scenarios, so the representation of different source characteristics is a relevant feature. The Y indicates that the model has separate modules for at least some different source representations. The B indicates that there is flexibility in the source representation, but that it is built into the general model structure, rather than as a separate module. The N indicates that separate source representations must be used before this particular model can be run.

In addition to these major model features, several other criteria should be considered in the choice of basis for the safety analysis model. Some of these involve physical process modeling, while others are less tangible and are concerned with actual implementation of the modeling upgrades. The

secondary features considered in the review are given below with no relative importance attached to the order.

12. Representation of aerosol dynamics

Although a UF_6 accident is likely to initiate with some release of liquid or vapor UF_6, it will rapidly undergo a phase change when exposed to standard atmospheric conditions to become a mixture of vapor and particles. The size composition of these aerosols can have an important influence on the subsequent evolution of the dispersing cloud. The optimum model would include some microphysics to control size distributions, and also represent the influence of aerosol size on downstream deposition. Some models make no attempt to include any aerosol dynamic effects.

13. Interaction with fog, precipitation, cooling tower plumes, etc.

Since it has previously been suggested that naturally occurring H2O aerosol clouds may interact strongly with a UF_6 plume (Hicks et al., 1985), it may be important to include the possibility of such an interaction. Certainly, the cooling tower plume at the edge of the plant along with numerous fogs along the Ohio river valley will present ample opportunity for a significant fraction of possible release scenarios to involve such interactions. None of the listed models attempt such an interaction.

14. Interactions with the ground

In simulating a dense gas which tends to hug the ground it is desirable to include a number of potentially important interactions with the surface. The leading edge of a gravity current can be made unstable by momentum transfer to the surface, heat transfer from the surface may be responsible for a pool of liquid on the surface boiling off, or the surface may provide moisture which can react with UF_6 and release latent heat when it is evaporated. The surface could be a water surface, such as a lake, or it could be a land surface with snow or ice cover, or simply a wet surface after precipitation or dew formation.

15. Ease of use

The ease with which a model can be used is important not only because it increases productivity, but also because it greatly reduces the chance for misuse. This includes both the clarity of the input/output interface and also the computer time required to make the calculation. Models which involve complicated initialization procedures are obviously more difficult to use and more susceptible to error. Rapid turnaround of results is valuable for the safety analysis application, where a wide range of parameters must be investigated. Long delays between runs increase the chance of error as continuity is lost from one calculation to the next.

16. Ease of modification

Since none of the available models satisfy all of the desired features for a safety analysis model, it will be necessary to modify the chosen model. The difficulties in modifying an existing model depend on the level of model complexity and modularity of the programming architecture. These aspects are very hard to assess from external review.

17. Agency acceptance

A safety analysis has two distinct purposes. First, it should provide management with a valid assessment of the safety of the operation, but it should also provide the public with an assurance that the assessment is indeed valid. It should be easier to accomplish the second of these if the model used has wide acceptance.

2.2 Model Evaluations

The models listed in Table 2.1 have undergone various degrees of evaluation. The best way of instilling confidence that a model can distinguish when any release will constitute a serious safety hazard is by testing the model in comparison with a variety of well controlled field tests. Unfortunately, existing evaluations have rarely if ever been made under sufficiently varied conditions to pass a rigorous statistical test. We believe that evaluations such as those carried

out in Hanna et al. (1991), and Hanna and Chang (1991), although very useful, generally imply a greater confidence in the models than is warranted by the actual test results.

There are at least two reasons why there is a built-in bias towards making the comparisons between field tests and model results appear unduly favorable. First, there is a strong tendency to filter out data that is hard to match with any models; and second, there is the equally strong tendency to keep varying some of the model's numerous input conditions until there is a reasonable match with the data. Fundamentally, both the experimenter and the modeler want the comparison to be favorable. This leads to the bias even when everyone is attempting to be scrupulously honest.

The evaluation bias problem is further compounded by the tendency for evaluation to be intimately connected with model development. Venkatram (1988), describing the attributes of model evaluation, says "Evaluation is a process in which the model is improved on the basis of the comparison between model predictions and observations. This interaction between comparison and model improvement will give rise to additional testing procedures. Therefore, model evaluation is an evolutionary process that is an integral part of the model development process". This comes close to assuring that no unfavorable evaluations will be reported, since any unfavorable result leads directly to a model modification. Granted this makes evaluation an essential part of model development, but it undermines the confidence that the model can provide accurate predictions for any untested conditions. It makes it difficult to distinguish whether any favorable comparison is a result of good model physics or simply good model tuning. In fairness to Venkatram, he does in his other attributes describe it as a series of tests to determine whether the model is an adequate representation of the real system being modeled, and says that the success of a model evaluation is critically dependent upon the scientific judgment of the model builders.

Figure 2.1 shows one of the summary result figures from Hanna et al. (1991) (Fig. 11, p. 127). The test data comes from the Thorney Island releases of dense gases (McQuaid and Roebuck, 1985), and the model results come from several of the models included in Table 2.1. The dashed line represents factor of two agreement between mean predictions and observations. It is readily seen that all of the models, except AFTOX and INPUFF, neither of which incorporates any dense gas effects, pass this factor of two agreement test. What is most surprising to us is that only DEGADIS shows any significant random scatter in the Geometric Variance VG = $\text{Exp}[(\ln Co/Cp)^2]$. This is indicated by the fact that the other model results lie close to the solid line which represents the

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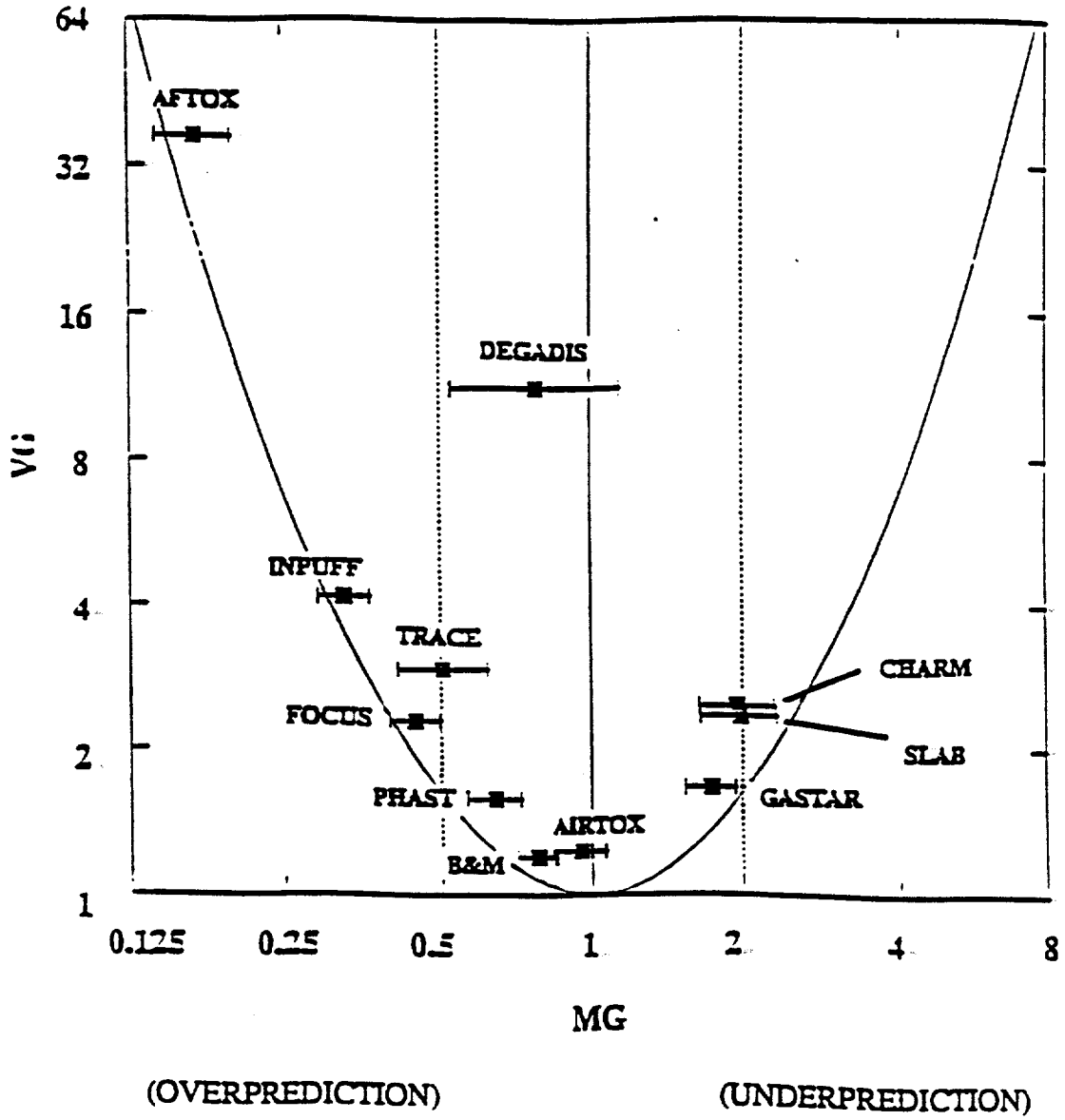


Fig. 2.1. Model performance measures, Geometric Mean Bias $MG = \exp(\ell nC_o - \ell nC_p)$ and Geometric Variance $VG = \exp(\ell nC_o - \ell nC_p)^2$ for concentration predictions and observations for the instantaneous dense gas data from Thorney Island. 95 percent confidence intervals on MG are indicated. The solid line is the "minimum VG" curve. The dashed lines represent "factor of two" agreement between mean predictions and observations.

variance caused by the indicated bias. We would expect considerable random scatter in the concentration data due to the inherent randomness of the atmospheric turbulence which would be expected to interact strongly with the dense gas dispersion. Why doesn't this randomness show up in the test results?

In an attempt to answer the last question, we investigated the data used in the comparison. Hanna et al. (1991) includes tables of the data used in their evaluation. They used data from 9 different instantaneous releases for the tests leading to Fig. 2.1. Data from 7 other tests were not used for some unspecified reason. The observations used all show a smooth falloff in concentration with increasing distance from 40 m to 583 m from the release point. We found no indication of what filtering of the data had been used to achieve such smooth data. A look into the data report by McQuaid and Roebuck (1985) shows that the original data contained a significant degree of both temporal and spatial variability. Insufficient detail is given to completely trace the filtering of the data, but it seems that the temporal and much of the spatial variability are eliminated by only considering the peak concentrations (averaged over 0.6 s) for each radial distance from the release point. This leads to a plot as given in Fig. 2.2 (Fig. 16.6, p. 163 of McQuaid and Roebuck) for each test case. This data appears to have undergone a further smoothing in the process of reducing it to the 5 points in the table of concentration versus distance used for this particular test case. These points are indicated by the check marks on Fig. 2.2. Of course it may be that further analysis of the raw data since 1985 has indicated that some of the roughness in Fig. 2.2 is due to faulty sensors and thus dropped, but it appears that only the points making up a smooth upper envelope are included in the data used for model comparison. This allows the data to agree with the modeler's bias that the concentrations should fall off smoothly with distance from the release point.

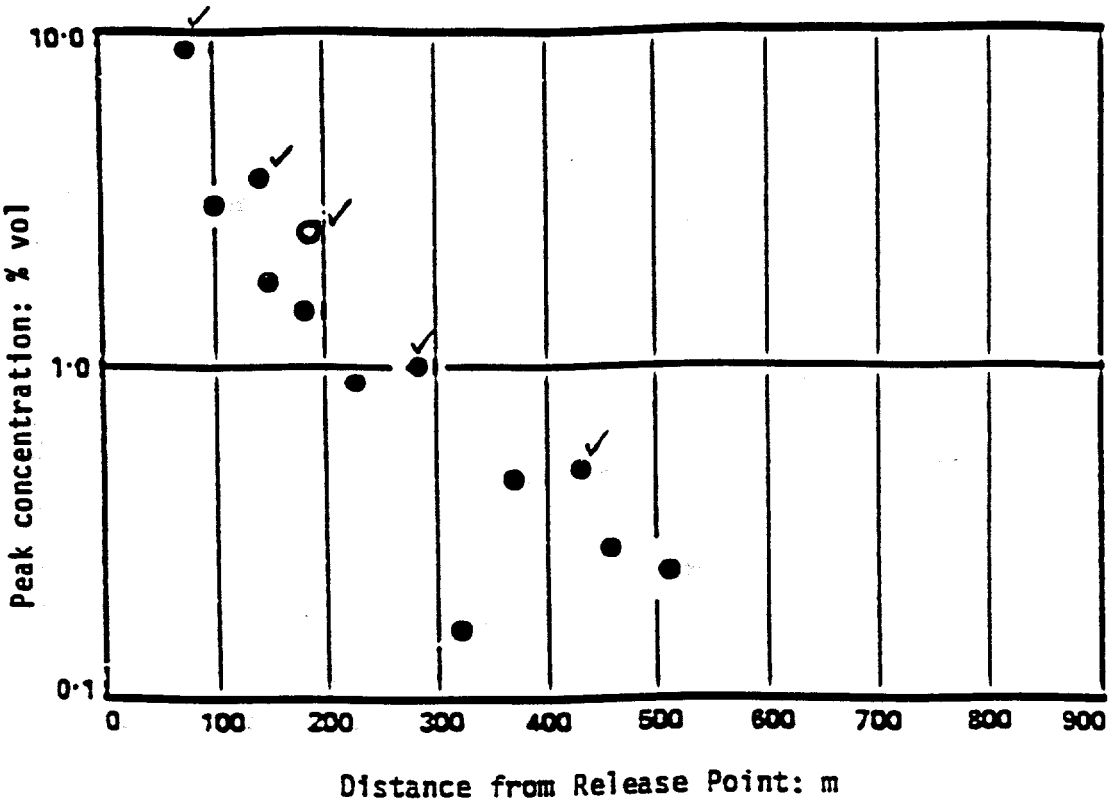


Fig. 2.2. Peak concentrations from all the sensors (solid circles) in the gas cloud at 0.4 m height. (Data from trial 006, Fig. 16.6, p. 163 of McQuaid and Roebuck).

As a result of our review of this evaluation we are not assured that the models have obtained the desired close agreement with observation as a result of good physics in the models. The model predictions of peak mean concentration versus distance have been compared with the observed peaks in concentration fluctuations versus distance. If the fluctuations were being correctly simulated by the model, we would expect the peaks in the observed concentrations at any distance actually to exceed the peak mean concentration at that distance. This may seem unimportant, but for the short times involved in sampling (0.6 s), we believe there could easily be a factor of 2 distinction between these measures. Thus, considering that the fluctuations about an ensemble mean have been ignored, the close agreement between model predictions and field observations presented in Fig. 2.1 may be as much due to model tuning as it is to model physics.

From our point of view, the seemingly high-scatter results for DEGADIS presented in Fig. 2.1 look preferable to the results presented for the other models. However, this scatter is not obtained as a result of considering any possible fluctuations, but rather seems to be the result of some strange comparison anomaly. Unless there is a typing error in Appendix C of Hanna et al., 1991, DEGADIS does not predict a smooth falloff in peak concentration with distance for 3 of the trials. Predictions for Thorney Island Trial 9 appear actually inverted with a smooth increase in peak concentration with distance from the release. It looks like the DEGADIS random scatter may be caused by some erroneous rise in the initial release or by some scrambling of the model results in the comparison process.

The most optimistic interpretation of this type of evaluation would be that the modeler has correctly adjusted the model to yield the local concentrations in the narrow high concentration ribbons of the plume, and that the experimenter has provided a sufficiently dense sampling network to capture these same high concentration ribbons. Then if the only data eliminated is on those arcs which were not able to capture the peak concentrations, we can take the evaluations at face value and give the models full credit for correctly predicting the peak concentration. However, we are skeptical and suspicious that much of the very favorable agreement that has been obtained between dense gas model results and field observations is illusory. This tends to undermine the apparent strong advantage of using an accepted dense-gas model as the basis for the desired UF_6 safety analysis model. Of course, in spite of this technical problem, the use of an accepted dense-gas model retains a strong public relations advantage.

2.3 Selection of Five Possible Candidate Models

None of the models listed in Table 2.1 satisfy all of the requirements for the desired UF_6 safety analysis model. Which ones are likely to form the best foundation for further development into a suitable model? Based on this broad screening of the models, we choose five models in this section for much more detailed scrutiny in the next section. Here we will only indicate why the particular model passes this first hurdle.

There are clearly a large number of models available for the prediction of dispersion of gas releases in the atmosphere, so we do not need to consider models that require very extensive modification. We first eliminate the models that have either no transient release or no continuous release capability (i.e., CRUNCH, DENZ, HEAVYPUFF, PLUMEPATH, TRAUMA, and TECJET) since the UF_6 problem requires consideration of both. We also eliminate the models with no dense gas capability and no other special qualification for the UF_6 problem (i.e., D2DC, AVACTA, INPUFF, RIMPUFF, SPILLS, SRI PUFF, SAFE, MESOI, and SCIPUFF). These models generally consider only positive buoyancy, and we consider it more straightforward to add this to a dense-gas model than adding dense gas effects to one of these models. We further require the model to have some independent validation if we are to consider modifying it for application to the UF_6 problem. This restricts the selection to the better known models, which are sufficiently well recognized to be tested against atmospheric data by independent researchers. We eliminate EAHAP, Eidswik, EPIDIS, CARE, MIDAS, ModSys, SAFEMODS, SAFETI, VAPID, and WHAZAN on this basis.

We further restrict the choice of models by eliminating the proprietary codes, CHARM and COBRA, since they do not demonstrate any significantly different capability to the public domain models. Their main advantages are usually found in the user interface, with increased attention to input formulation and flexibility of output, but the public domain models have been more widely applied and tested, in general. None of the models can be directly applied to the UF_6 safety analysis problem, so the difficulty of access to the proprietary codes makes them less desirable as a starting point. Any model development would most likely require the assistance of the code developers, and while this may prove to be the most effective method even for the public domain codes, it is much easier to achieve outside the encumbrances of a proprietary framework.

We also eliminate the three-dimensional fluid codes, represented in Table 2.1 by FEM3A only. FEM3A is one of the best examples of a hydrodynamic prediction code for dense gas cloud behavior (see the review by Havens et al., 1987), and provides the most rigorous model for the fluid mechanics. It does not need to make assumptions about cloud shape or the interaction between the buoyancy and momentum fields, but it does use turbulence model assumptions. The major difficulty with its use as a safety analysis model lies in the complexity of initialization, the expense of the computation, and the limitation in lateral scale of the calculation. The scale limitation is imposed by the need to resolve the entire flow field on a three-dimensional net of elements, so FEM3A is best suited to the study of a local region of the flow. It is extremely difficult to design a net that resolves

the narrow plume close to the source, but that also extends out into the far field to represent the concentration field accurately at distances of several kilometers. The three-dimensional model also requires a complete specification of the atmospheric velocity and temperature field for the calculation, and the model must be run long enough for the flow to reach equilibrium in the presence of any terrain or buildings. FEM3A does not contain any UF_6 chemistry. We consider FEM3A to be valuable as a research tool for the study of detailed dynamic behavior, from which parameterizations can be derived for use in the simpler models.

PLM89A is included as a candidate model at this level for two basic reasons. First, it starts with the most complete UF_6 chemistry of any of the available models; and second, it will probably be the easiest for the personnel at Energy Systems to modify, since they developed it. PLM89A has already received a critical review, and several deficiencies have been pointed out. The task of the present review is to determine the level of effort required to remedy these deficiencies compared with the development of an alternative model. We must additionally consider the potential advantages of an alternative model (e.g., improved capability in various areas).

TRIAD is included because considerable effort was expended in an effort to develop this model for exactly this application when the Energy Systems model (effectively PLM89A) was deemed inadequate in 1985. TRIAD is based on three existing models, combined within a single framework for application to the UF_6 dispersion situation. The submodels are EPA's INPUFF dispersion code, a wind field interpolation scheme from MESOI, and a simplified representation of the UF_6 chemistry from PLM89A. The model does not meet all the requirements of the safety analysis model, but its shortcomings will be considered relative to the other candidates.

The preceding two models, PLM89A and TRIAD, are the only codes designed to predict UF_6 dispersion that we are aware of. There are a wide range of alternative dispersion models, but we have focussed on the dense-gas models since this is such an important aspect of the UF_6 release. Almost all the models in this category contain a transition to the passive dispersion phase, and therefore meet two of the safety analysis requirements immediately (i.e., zero and negative buoyancy dispersion). SLAB (Ermak, 1990) is one of the more widely accepted dense gas models, having "passed" numerous evaluation tests, and is therefore included as one of the candidate models. It treats a wide range of buoyancy conditions and source types, and is readily available.

ADAM (Raj and Morris, 1987; Mullett and Raj, 1990) was developed for the Air Force for the prediction of hazardous chemical releases. It is included as a candidate model for the UF_6 safety analysis because it has a general chemistry package added to a dense gas dispersion model. Several different chemical reaction schemes have been incorporated into ADAM's framework, and the most relevant for the current application is the description of an HF release. ADAM was developed to simulate accidental releases and contains a useful range of source descriptions. The model has been evaluated against a number of dense gas experiments, and shows reasonably good predictive capability.

The final choice for inclusion is HGSYSTEM (McFarlane et al., 1990; Puttock et al., 1991, Witlox et al., 1990) because this package of models also describes the behavior of HF, one of the major components involved in the UF_6 safety analysis. It also includes a HEGADAS dense gas dispersion module, and different source modules. HEGADAS (Witlox et al., 1988) is one of the widely accepted dense gas models, comparable to SLAB, and has been extensively evaluated against atmospheric test data. The models were developed under the sponsorship of several oil companies, but are available for general use. DEGADIS (Havens, 1988) is the other well-known public-domain dense gas model, but is closely related to HEGADAS. We therefore only consider HGSYSTEM for the UF_6 application, in preference to HEGADAS and DEGADIS, since it contains the framework for the chemical reactions.

3. DETAILED REVIEW OF CANDIDATE MODELS

3.1 Atmospheric Dispersion

The ambient atmospheric dispersion will always dominate the plume transport and dilution sufficiently far downstream. The point at which the plume dynamics become negligible in comparison with the ambient turbulence levels will depend on the source characteristics, but a reasonable representation of the transport and diffusion by the prevailing wind field is a vital part of the safety analysis model. There are two parts to the description of the local atmospheric effects. First, the state of the atmosphere must be specified (i.e., the wind, turbulence fields, and thermodynamic state), and second, the plume behavior in the atmosphere must be modeled. The approaches used in the principal candidate models are reviewed in this subsection.

3.1.1 PLM89A

The current Energy Systems model uses the empirical Pasquill-Gifford-Turner (PGT) stability categorization to describe the atmospheric conditions. This allows the local conditions to be specified by a wind speed and a stability class (i.e., a relatively low-dimensional parameter space which has the advantage of being easily surveyed to determine 'worst-case' conditions). The ambient plume spread rates are then determined from empirical power law relations, in the form

$$\sigma = A\chi^b$$

where σ is the plume spread (vertical or horizontal), χ is the downstream distance, and A and b are constants that depend on the stability. Different constants are used for vertical and horizontal spread rates. PLM89A uses an effective origin to shift the PGT curve to match the dynamically-generated plume spread at each downstream location, so that a smooth transition to the ambient spread rate is achieved. This transition is provided for the plume area only, rather than separately for horizontal and vertical spreads. PLM89A contains an adjustment in the horizontal spread rate to account for different sampling times, using a power law relation to reduce the lateral spread for sample times less than 10 minutes. An instantaneous concentration measurement is defined as an 18.75-s time average.

3.1.2 SLAB

The atmospheric profiles in SLAB are based on surface layer similarity theory, and therefore use dynamically relevant parameters. Detailed velocity profiles are constructed in terms of surface friction velocity, surface roughness length, Monin-Obhukhov length, and mixed layer depth. The profiles are extended throughout the depth of the mixed layer to provide a complete description of the mean wind. Turbulent diffusion rates in the vertical direction are also based on these profiles, but are combined with the dynamic perturbations due to the plume itself in a complicated parameterization. The ambient contribution uses turbulence intensity estimates based on surface friction velocity and stability with composite profiles to represent the surface layer and the complete mixed layer. Horizontal diffusion rates are also based on a sample averaging time, which recognizes the meandering nature of the plume in the near source region. The spread rates are matched to the PGT predictions for a nominal 15 minute averaging time, but are reduced for shorter times using a simple power law.

The boundary layer parameters in SLAB are deduced from a specification of the PGT stability class so that the model can be used with the standard type of input for atmospheric diffusion models. Monin-Obhukhov length covers a reasonable range with a dependence on surface roughness length. However, the boundary layer height is set equal to 130 m for stability F and doubles for each class change (i.e., 260m for E, 520m for D). This arbitrary specification ignores the large variability in mixing depth for any particular stability. A similar arbitrariness is introduced in the lateral velocity fluctuations, implicitly included in the definition of the lateral entrainment velocity. This also depends only on stability class, except for its proportionality to the wind speed, and again ignores the large variability.

3.1.3 HGSYSTEM and ADAM

These two models both use similar concepts to SLAB for the vertical diffusion, but are simpler in implementation. The velocity profile is specified in terms of surface layer parameters, and appears to be restricted to surface layer diffusion, consistent with the models' use for dense gas prediction. Horizontal diffusion in both models is still based on the PGT stability category, using the usual empirical power law relations.

3.1.4 TRIAD

TRIAD provides the option of using either the PGT scheme (similar to PLM89A) or an on-site scheme (using local meteorological observations). The PGT scheme is augmented slightly by dividing the neutral D-category into two subcategories, as suggested by Pasquill (1961). The two classes are referred to as D-day and D-night. The dispersion schemes in TRIAD are obtained directly from EPA's INPUFF model (Petersen and Lavdas, 1986).

If on-site meteorology is used, the spread rates are determined from estimates of the r.m.s. velocity fluctuations in the horizontal and vertical. In addition, an estimate of the time correlation is needed; and this is specified as a simple algebraic function, following Irwin (1983). This specification gives a timescale of 1000 s for horizontal fluctuations and infinity for vertical fluctuations under unstable conditions. The latter assumption is not unreasonable, since the plume will rapidly fill the mixed layer and further diffusion will be limited. For stable conditions, a 50-s timescale is assumed. TRIAD also suggests values for the velocity fluctuations as a function of stability category,

so that the on-site method could be used with only a mean wind and PGT class as input, following Gifford (1976) and Hanna et al., 1982. Use of these PGT-derived values is not recommended in the TRIAD documentation, since the fluctuation levels can be very different in complex terrain and/or light wind conditions.

TRIAD also provides a user-controlled option to switch the dispersion rate to a late-time value, where the puff grows at a rate proportional to the square root of time. This feature is activated if the puff size exceeds a specified criterion. However, the utility seems very limited, since the standard algorithms automatically provide square root growth at late time. The user must have specific knowledge about the local dispersion phenomenology to override the standard INPUFF values.

3.1.5 Recommended Improvements

All the candidate models, except for SLAB, use the empirical PGT relations for the ambient horizontal atmospheric diffusion rates. The main advantages of the PGT scheme are its quantization of meteorological conditions, and its established position in atmospheric dispersion modeling. The disadvantages of the scheme include the difficulty in specifying the actual stability class for real conditions and the limited ability to describe the true complexity of real diffusion. The turbulence structure in the atmospheric boundary layer cannot be properly described simply in terms of wind speed and a stability category. The empirical PGT dispersion curves were generated for relatively short range surface releases of passive tracer, and they do not adequately describe the nature of the turbulent flow fields in the atmospheric boundary layer. Our current state of knowledge allows a much better description of the turbulent diffusion (Weil, 1985) in terms of the important boundary layer parameters, such as surface friction velocity, surface heat flux, mixed layer depth. However, the stable boundary layer is still not well understood and is probably very dependent on local terrain features which require site-specific models. The PGT scheme has some rational basis as a representation of surface layer dispersion over relatively short range, where stability and wind speed are the controlling parameters, but needs to be embedded in a more systematic treatment of turbulent diffusion.

The safety analysis model should utilize a representation of turbulent diffusion in the atmosphere based on our current understanding of the phenomena. There are two distinct types of

dispersion to be considered, namely absolute and relative dispersion. Absolute dispersion is appropriate for a long term average of the plume from a continuous source, while relative dispersion measures the spread about the cloud centroid and ignores the meandering component of the wind. Relative dispersion is more appropriate for an instantaneous estimate of concentration values. Both rates of diffusion are controlled by the velocity fluctuations, but different scales of motion are involved in the two types.

For absolute diffusion, the rate of spread of the concentration field can be directly related to the turbulent velocity fluctuation correlations if the fluctuation correlation timescale is known, using Taylor's (1921) result. These relations were framed within the context of turbulence closure models by Sykes et al. (1984), and the relationship was incorporated into a Gaussian plume framework (Sykes et al.,1986). The PGT scheme is more appropriate for relative dispersion, however, since the large-scale meandering motions cannot be described in terms of surface layer parameters; and we believe that a rational connection to surface layer turbulence estimates can be made for the PGT classification scheme. The dispersion parameterization in SLAB goes part of the way toward the objective of relating dispersion to measurable turbulence quantities and maintaining the link to PGT stabilities, but it does not maintain an explicit description of the turbulence intensities and timescales. We therefore recommend a more complete description of the turbulence.

There are several advantages in recognizing the relationship between turbulent velocity fluctuations and the dispersion process. First, the use of velocity variances in the spread prediction allows the model to use measured turbulence levels, if they are available, otherwise turbulence estimates based on alternative measurements must be used. Part of the difficulty in adopting an improved scheme requiring turbulence input data lies in providing this input, and therefore a rational connection with the PGT stability classification is desirable for the early application of an advance scheme. However, decoupling the specification of the turbulence from the diffusion relationship permits the turbulence inputs to be upgraded as better atmospheric flow measurements become routinely available. These measurements are important in defining site-specific flow conditions, and can only be utilized in a model that relates these measurable quantities to the diffusion rates. The second advantage is the ability to describe the effects of averaging time in a rational manner, since we have an explicit model for the fluctuation statistics. These effects are important for the chemical reaction processes and also for assessment of hazardous effects, which may depend on short duration exposures.

The basis of the advanced scheme will be a relationship between the atmospheric turbulence profiles and the plume dispersion rate. Plume spread rates can be written in the form of an entrainment velocity for inclusion in the candidate models. A simplified representation for absolute diffusion that does not require any additional variables to be computed by the code can be written, following Ermak's SLAB implementation, as

$$\frac{d\sigma_y}{dt} = \frac{\sigma_v}{1 + \sigma_y/\Lambda_h} ,$$

where σ_v is the r.m.s. lateral velocity fluctuation, $\Lambda_h = \sigma_v\tau_h$ is the horizontal turbulence length scale, and τ_h is the integral timescale. This representation matches Taylor's (1921) analytic result at early and late times, and is therefore valid for the ensemble average spread of a cloud. The transition from early to late time can be achieved with a variety of functional forms for the denominator; only the asymptotic forms are specified by the theoretical match. A similar relation can be used for the vertical spread rate in terms of the vertical velocity variance. However, it is more appropriate for the safety analysis to use a relative diffusion estimate, which can be very simply modeled by replacing σ_v in the spread rate equation with

$$\hat{\sigma}_v = \begin{cases} \sigma_v \left(\frac{\sigma_y}{\Lambda_h}\right)^{1/3} & , \sigma_y \le \Lambda_h \\ \sigma_v & , \sigma_y > \Lambda_h \end{cases} .$$

This formulation only uses the turbulence energy on the scale of the instantaneous plume for a small plume, scaled down from the total fluctuation intensity using the Kolmogorov spectral power law. For larger scale plumes, the instantaneous spread grows like the ensemble average spread. This gives a $t^{3/2}$ growth at early time and $t^{1/2}$ growth at late time. Vertical diffusion can be represented by a similar formula using σ_w and τ_z or Λ_z.

The atmospheric vertical velocity fluctuations can be specified in terms of u_* and the convective velocity scale, w_*, defined by the relation

$$w_*^3 = \frac{gH_0 z_i}{T_0} ,$$

where T_0 is the reference temperature, z_i is the mixed layer depth, and the surface heat flux, H_0, is in velocity units. Convective scaling only applies for unstable conditions (i.e., positive heat flux). However, for neutral and stable conditions, the vertical velocity variance is also readily specified in terms of u_* and the Monin-Obhukhov length, L. Details of a proposed representation for the atmospheric turbulence and the dispersion rates in terms of boundary layer parameters is given in the appendix. The functional forms for the profile assumptions are described there, and some results for actual dispersion rates are included. The scheme is simple enough to be implemented in any of the Gaussian-type dispersion models, and a practical connection with the standard PGT stability categories is included to allow the scheme to be used with conventional boundary layer input data. The scheme provides a realistic means for predicting time-average exposure and instantaneous plume spreads for use with the nonlinear process models.

3.2 Dense Gas and Dynamic Effects

The UF_6 model must be capable of simulating the effects of a denser-than-air release, since UF_6 is much heavier than air at ambient temperatures. It is possible that the heat and HF produced by chemical reactions could reverse the buoyancy effects, but the model still needs the dense gas capability for UF_6. This capability is also important for other hazardous materials of interest to the Department of Energy.

There are three phases where the negative buoyancy effects may be important. The first is in the airborne phase of a jet or elevated release, during which the trajectory of the plume is directed downward toward the ground. The second phase is the "ground hovering" regime, where the plume is constrained from further downward motion by the ground. In the second phase, the gas tends to spread along the surface like a pool due to the pressure gradients produced by the increased density in the middle of the plume. The third phase is after the horizontal spread due to pressure gradients is halted, but there is still a stabilizing effect of the density gradient on vertical diffusion induced by atmospheric turbulence. The treatment of these effects in the major candidate models is reviewed below.

3.2.1 PLM89A

The jet phase is modeled by PLM89A using conservation of buoyancy and vertical momentum to predict the plume trajectory. The model can describe elevated sources with momentum and buoyancy. The jet entrainment is modified for stability effects, and is strongly reduced under conditions of significantly negative buoyancy. However, under these conditions one would expect the plume to reach the ground relatively quickly.

Once the plume centerline has reached the surface, it becomes a ground-hovering plume, and the gravity spreading term is activated. This is a lateral spread term, based on the hydrostatic pressure gradient across the plume induced by the density gradients, and is similar to most of the dense gas spread rates. The lateral spread is not diffusive, since it is associated with a vertical "slumping" of the cloud, and this conservation of area is ensured in PLM89A by use of a separate area computation. The increase in area is due only to entrainment processes, either by plume-induced turbulence or ambient atmospheric turbulence, and the vertical extent of the cloud is deduced from the predictions of the area and the lateral spread.

The turbulent entrainment is modeled as either a jet-related value or the ambient value obtained from the stability-dependent Gaussian plume dispersion rates. These rates are based on the Pasquill-Gifford-Turner stability categories with an appropriate plume origin, and are discussed in more detail in Section 3.1. Transition to the PGT entrainment model occurs whenever the jet entrainment falls below the ambient Gaussian value. The ambient atmospheric entrainment will quickly dominate the ground-hovering plume since the jet velocities will decrease rapidly as the plume

spreads and slows down. In any event, PLM89A does not properly account for the reduced entrainment caused by the stable interface between the plume and the overlying ambient air in terms of the local Richardson number. This is a serious deficiency from the point of view of safety assessment since the suppression of vertical diffusion could maintain high-concentration values in the cloud for significant downstream distances.

3.2.2 SLAB

SLAB is specifically designed to model dense gas spills, and therefore uses parameterizations specifically designed for such flows. SLAB uses two modes to simulate a general entrainment release. A steady state plume mode describes the evolution during the release with transition to a puff mode at the end of the release. Note that the release rate must be constant over the period of the release.

SLAB models source jet effects, horizontal or vertical, or an evaporating pool using the steady plume assumption. An explosive release could be modeled as an instantaneous puff. The treatment of dense gas effects in SLAB is similar to the other spatially-averaged dense-gas models, and is more sophisticated than the PLM89A model.

First, SLAB uses two lateral spread measures to distinguish between gravity spreading and lateral diffusion; the gravitational spreading is based on the van Ulden (1984) correlation. This information is used to determine the crosswind concentration distribution which is nearly uniform if gravity spreading dominates. Differences from a sample Gaussian are perhaps as large as a factor of 2, and may not be critical for the UF_6 safety analysis requirement, given the large uncertainties in other aspects.

The second major difference is in the entrainment model, where SLAB uses plume stability parameters to control the mixing rate. This allows plume density effects to reduce the vertical entrainment in a realistic way, and provides a smooth transition to an ambient atmospheric value as plume buoyancy becomes negligible. The ambient atmospheric values are based on surface layer turbulence concepts, with appropriate definitions in terms of stability classification if the user prefers. The entrainment rates are obtained from relatively complicated parameterizations, based on combinations of ambient turbulence levels, ambient stability, plume velocity, length, and density scales. The parameterizations are designed to model the effects of shear-induced turbulence (both shear due

to flow over the surface and shear between the plume and the free atmosphere) and the stabilizing effects of the density gradients.

SLAB also includes surface heat transfer and phase change between liquid water and vapor with associated latent heat transfer. SLAB does not contain chemical reaction, but the inclusion of water components suggests that exothermic reactions would not be very difficult to include in this framework.

3.2.3 HGSYSTEM and ADAM

The treatment of density effects in these two models is similar to SLAB, although the details of the entrainment parameterization are different and significantly simpler. The gravitational spreading term is modeled in the same way as PLM89A , using the van Ulden (1984) relationship. The atmosphere is characterized in terms of a surface friction velocity and a Monin-Obhukhov length, and this provides the ambient vertical diffusion rate, which can be expressed as an entrainment velocity. This rate is modified for the dense cloud using a function of Richardson number, defined in terms of the plume density difference, the ambient friction velocity , and the depth of the plume. This representation is considerably simpler than the expressions used in SLAB, but does not contain the same level of generality. Use of the ambient friction velocity as the only turbulence scale implies that the plume velocity scales are negligible, so some enhancement of this value should be included to describe low wind speed cases.

HEGADAS uses a reduction factor of the form

$$\frac{1}{(1 + 0.8\ Ri)^{1/2}}$$

for dense clouds. HEGADAS also contains a parameterization for positive buoyancy in the cloud. ADAM uses a factor

$$\frac{1}{(a + b\,Ri^2)^{1/2}} ,$$

but the values of a and b are not specified in the documentation for ADAM, and only negative buoyancy is accounted for. The Richardson number is simply defined using the plume density excess, the plume depth, and the turbulent friction velocity.

The latest version of HEGADAS used in HGSYSTEM also has a transition to a lower gravitational spread rate when the leading edge of the gravity current becomes sufficiently turbulent.

3.2.4 TRIAD

TRIAD contains no representation of dense gas effects and only has a very limited dynamic capability. TRIAD does contain a plume rise prediction, based on source momentum and buoyancy, but this is in the form of a standard plume rise formula (Briggs, 1969, 1971, 1973, 1975) and is used to determine the effective source height for each puff. The effective plume rise is computed for the given source and puffs are released at the final height, so the rise process is essentially parameterized as part of the source specification. This approach is justifiable for simple sources if the interest lies in the concentrations far downstream of the rise phase, but is not adequate for the UF_6 problem where the dynamics and chemistry interact in a complex manner in the early plume.

3.3 Transient Release Effects

A safety analysis model must consider a number of possible release scenarios, some of which are quasi-steady while others are short duration or near instantaneous. Many of the available dispersion models can deal with a range of sources, but the spatially-integrated Gaussian-type models all have some restriction. A fully three-dimensional, time-dependent dynamic flow model can clearly treat unsteady sources, but we believe such models to be impractical for the current application.

The current Energy Systems UF_6 model, PLM89A, is basically a steady-state plume calculation, but transient release effects are modeled by applying a translating "window" function to the plume result. This window includes streamwise diffusion effects, and gives a reasonable estimate of the translation and diffusion effects on the mean concentration at any downstream location. However, as noted in the model description (Bloom et al., 1989) and in the review of Hicks et al. (1985), the window function only applies to the species concentrations after the plume calculation has been made. No account of transient effects on the nonlinear dynamics and chemistry is taken, making the transient solutions from PLM89A unreliable.

The TRIAD model provides the most detailed treatment of transient releases through its representation of the cloud as a series of Gaussian puffs. Each puff can be released with a different mass of UF_6 so that a time-dependent source can be modeled. However, TRIAD does not represent any dense gas effects, nor the effects of a transient release on the buoyant rise. The reduction in rise for a short duration or instantaneous release is not accounted for. The proper treatment of such effects would require, at a minimum, some calculation of the interaction between adjacent puffs and introduces significant complexity into the puff computation. This method was employed in the SCIPUFF code to represent buoyant rise of a series of puffs from a power plant stack (Sykes et al., 1988).

The dense-gas models (SLAB, HGSYSTEM, and ADAM) all have techniques for dealing with transient sources. However, the models are constrained to run as either a plume calculation or as a three-dimensional puff calculation. The technique in SLAB is to represent the source as a plume while material is being released, then switch the finite-length plume over to a puff calculation for the remainder of the calculation. Instantaneous sources can be initialized as a puff, and the dense gas spreading in both horizontal directions is included. ADAM is basically restricted to treating either a steady plume source or an instantaneous release. The HEGADAS model in HGSYSTEM is also restricted to continuous steady releases. Unsteady emission rates are treated as a source variation, and an appropriate filter function applied to obtain an unsteady solution at any downstream location. This is roughly equivalent to the PLM89A treatment of

unsteady effects, except that HEGADAS includes contributions from both wind shear and gravitational spreading to streamwise diffusion.

The state of the modeling is such that the current dense-gas models have a slight advantage over PLM89A in their ability to deal with an instantaneous source. However, the need for treatment of transient buoyant jets and chemistry makes it worthwhile studying possible extensions of the Energy Systems model methodology to describe transient dynamics and chemistry.

Most of the nonlinear processes in a spatially-integrated model are treated by means of a "typical" plume value for the various quantities involved. For example, the vertical motion of the plume centroid is specified by the plume vertical velocity component, which is derived from a conservation equation for the spatially-integrated vertical momentum. If a correction for streamwise inhomogeneity, similar to that used for the scalar concentration, can be applied to these dynamic processes, then a reasonably consistent transient release model could be developed within the current Energy Systems framework.

Estimates of in-plume parameter values is relatively straightforward, since the three-dimensional integrated conservation laws are similar to plume conservation laws, so the same factor as used for the scalar concentration can be used. Thus, estimates of cloud velocities and concentrations used for centroid motion, entrainment parameterizations, or chemical reaction rates should be multiplied by a factor, ϕ_t, to account for transient effects. The factor, ϕ_t, is obtained from the general scalar concentration shape function $\phi(S_1,S_2,S_3)$ as defined in Sect. 3.3 of Bloom et al. (1989). While the release is in progress, we use the plume values and ignore transient effects, so $\phi_t = 1$. After the release has ended, however, we use a shape factor appropriate for the center of the puff (i.e., at the position $x_c = x(t-\gamma/2)$ where t is the time since initialization of the release and γ is the duration of the release).

Using the notation of Bloom et al., 1989, we have

$$\phi_t = \begin{cases} 1, & S_1 < S_2 \\ 1/2\phi(S_1, S_2, S_3), & S_1 > S_2 \end{cases}$$

where $S_1 = \frac{X_t}{A_x}$, $S_2 = \frac{X_Y}{A_x}$, $S_3 = \frac{X_c}{A_x}$.

Application of the ϕ_t -correction will account for transient effects in a number of processes, but it must be emphasized that the scale factor has to multiply the perturbation from ambient values. The calculation of A_x, and the dense-gas spreading effect in a ground-hovering plume need further consideration since the density induces streamwise effects other than simple diffusion. We should also emphasize at this point that the shape-factor technique is only valid for a finite-duration source with fixed characteristics, since the entire evolution is still determined by a single local description. This should not be a significant restriction for safety analysis since detailed transient source variations are not generally available. A complex release scenario, perhaps involving a short-duration, high-emission rate followed by a long term slow leak, would have to be modelled as separate releases with the proposed methodology.

The expression for A_x must include terms to represent growth due to

1. ambient atmospheric diffusion,
2. plume dynamical entrainment, and
3. gravitational spreading.

The model for A_x given by Bloom et al. (1989) assumes isotropy in the horizontal plane so that $A_x = A_y$. We believe that this simplifying assumption is justifiable for the safety analysis application, although some of the streamwise diffusion mechanisms are different from the transverse processes mainly due to the different shear profiles in the two directions. If the model does not use a sophisticated description of shear effects, then there is little reason to distinguish between the lateral and streamwise spreading rates.

It is desirable to formulate an evolution equation for A_x (and A_y) in the form

$$\frac{dA_x}{dt} = T_{entrainment} + T_{density}.$$

The entrainment term will be the same as that in the lateral spread equation, and should ideally include both ambient turbulence and plume turbulence effects. The prescription in the SLAB model provides an attractive scheme.

The density term will also be the same as that in the lateral spread, but proper account of the mass conservation due to streamwise gravitational spreading needs to be taken under consideration. The gravity spreading is different from diffusive spreading since it only involves a change in plume geometry. No mixing is implied in the term, so the cross-sectional area (or volume in three dimensions) should be unchanged. This is automatically satisfied in PLM89A for a plume since the area increase contains no gravitational term, and the vertical plume spread is deduced from the area and the lateral spread.

With the current methodology (i.e., an area prediction plus a lateral spread), the area equation would need to include a reduction term to account for streamwise gravitational spreading. Thus, to conserve volume, an extra term

$$\frac{d\theta}{dt} = - \frac{\theta}{A_x + L_x} \cdot T_{density},$$

where L_x represents the length of the plume, needs to be added to the mass conservation equation.

The inclusion of these streamwise dispersion terms does not give a complete description of a general transient source, but we believe that the representation of a constant rate, finite duration source would be as reliable as any of the other available methods except for full dynamic models.

3.4 Building and Terrain Effects

Buildings are generally present in the neighborhood of an accidental release, since this usually involves some type of storage facility. The UF_6 release scenarios envisioned for the current study take place on sites with very large buildings, so the flow modification due to the local structures is likely to be significant.

There are two major phenomena induced by building flows of relevance to the dispersion of hazardous materials. The first is the flow separation and increased turbulence in the wake of an isolated building, and the second is the channeling effect along the 'streets' between adjacent buildings. Since the buildings on the Paducah and Portsmouth sites are so large in comparison with the anticipated source and early time plume dimensions, some account of their effects should be included in the safety analysis model.

PLM89A does not represent any building effects, nor do the public-domain dense gas dispersion models, with the exception of FEM3A which represents structures explicitly in the three-dimensional calculation. Several of the proprietary models contain a building wake description, but we do not have a complete description of the parameterizations. We presume they are similar to the Gaussian coefficient modification suggested by Huber and Snyder (1982) and Huber (1984), and we will discuss its implementation below.

None of the models, except for the three-dimensional hydrodynamic models, describe the channeling effect of the buildings, even though this could be a very important effect for a dense gas spill in the neighborhood of large structures; so we also discuss a simple method for the description of this phenomenon.

For a source in the lee of a building, or upstream of an isolated building, the major effect of the increased turbulence is a rapid dispersion of the plume material. Huber (1991) presents comparisons of Gaussian plume estimates with wind tunnel data. The simple parameterizations provide reasonably good predictions, although the results are only valid for downstream distances greater than 3H, where H is the building height. The principal result of the building-induced flow disturbance is to generate a plume width of about 35% of the building width at $x = 3H$ and to give an effective origin shift for the standard Gaussian diffusion formulation so that σ_y at $x = 10H$ is equal

to 0.35W + 0.5H where W is the building width. Similar adjustments are recommended for the vertical diffusion.

In the context of the UF_6 safety analysis requirement, the isolated building assumption is unrealistic and also the release is not passive. The complex layout of the plant, and the buoyancy effects in the UF_6 release will make the plume behavior much more complicated. A simple representation of the turbulence enhancement can be achieved by use of an increased surface roughness length, if the turbulence parameterizations depend on roughness. The increased roughness is a measurable phenomenon and is readily justifiable. If the model does not utilize a surface roughness prescription, then a conservative approach to the modeling would be to neglect the enhanced diffusion due to the buildings and account only for their confining effects.

The channeling of the flow along the "canyons" between the large buildings can only be represented in a crude way. The details of the flow are extremely complex, but a very simple method of including the broad effect is based on limiting the lateral diffusion in the neighborhood of the buildings. This is the method used in the Gaussian model VALPUFF (Tangirala et al., 1992) for dispersion in deep valleys. The VALPUFF implementation restricts the lateral spread, σ_y, to be less than or equal to the valley width at the height of the plume, as illustrated in Fig. 3.1. This scheme could easily be adapted to represent a building "canyon" by limiting σ_y to the inter-building spacing whenever the plume is below the building height. This restriction would only be applied within the range where buildings dominate. Once outside the site, building effects would be dropped.

Beyond the range of the on-site buildings, the model may need to account for terrain channeling effects. There are some local valleys in the neighborhood of the Portsmouth plant. The VALPUFF methodology can be included in the safety analysis model by determining the appropriate limits for the lateral spread as a function of plume height from the terrain maps. We should emphasize that the plume width is only restricted from growing larger than the terrain or building limitation (i.e., if it is already larger than the restriction then it is not reduced, but it does not increase). The rationale behind this is that the flow itself is channeled through the valley or building canyon and therefore accelerates. The flow is incompressible and cannot increase local concentrations by channeling, so the spread cannot be reduced.

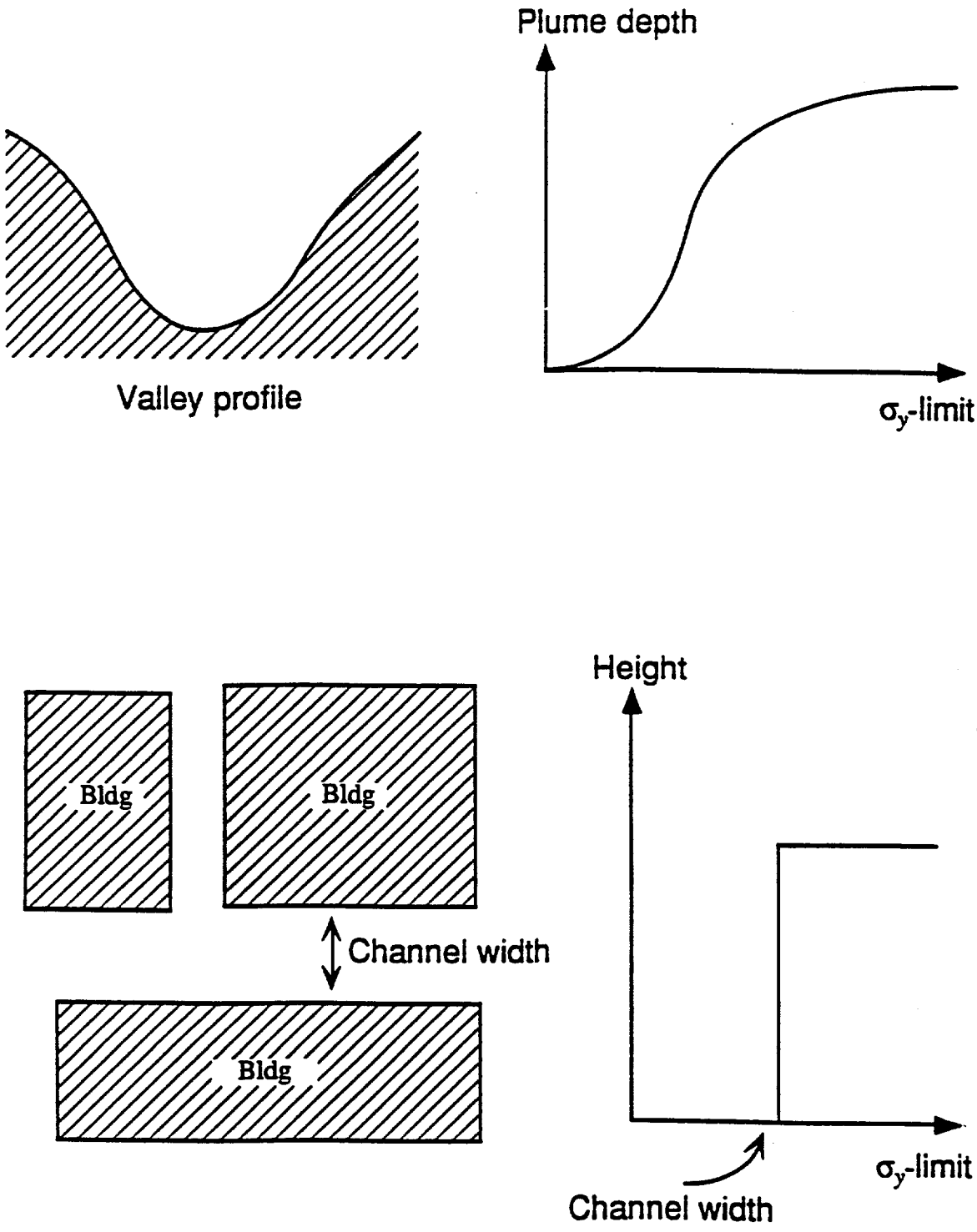


Fig. 3.1. Schematic illustration of lateral spread limits for terrain and building effects.

3.5 Chemical Reaction Effects

The safety analysis model must represent the chemical transformation of UF_6 into secondary components, and the subsequent reactions of these species. The reactions are complicated and exothermic, involving a number of species including water. The chemistry of UF_6 is very specialized, and is not easily accommodated in a simple, generic reaction scheme. In our review of available models, we have found no other dispersion model containing a description of UF_6 chemistry, although a framework for describing complex chemistry using UF_6 as an example has been presented in LLNL report and Rodean (1991). Rodean's scheme has not been incorporated into any dispersion model, however, so there are no immediately available models other than PLM89A and TRIAD with UF_6 chemistry.

There are, in fact, very few models containing a description of reactive components, and amongst our selected candidate models only ADAM and HGSYSTEM have this capability. ADAM has been developed to simulate a number of hazardous chemicals, including HF in a recent extension of the model (Raj, 1990). HGSYSTEM has been specifically designed to simulate HF releases. The description of the chemical composition of the plume in both HGSYSTEM and ADAM is achieved through solution of the local equilibrium equations (Schotte, 1987), assuming that the constituents are perfectly mixed throughout the cloud and that all reactions proceed rapidly. The solutions depend on the thermodynamic state of the cloud as well as the initial composition and entrainment components. These assumptions are consistent with Rodean's methodology, so that it seems possible that Rodean's description of UF_6 chemistry could be incorporated into ADAM.

In contrast to this method, PLM89A uses a finite-rate reaction scheme to describe the chemical evolution of the cloud, although an equilibrium option similar to Rodean's scheme is available. PLM89A contains a full description of the UF_6 chemistry, as well as it is currently understood. One minor criticism of PLM89A's chemistry in the review by Hicks et al. (1985), although perhaps of significance for the dispersion prediction, was the neglect of latent heat of evaporation of water droplets by the exothermic reaction between UF_6 and water. Thus, in a fog situation with plenty of water available for formation of HF, PLM89A might overestimate the tendency for the cloud to lift off the ground as it heats up from the reaction energy release. If a significant fraction of the energy was absorbed by the evaporation of the water droplets, the cloud

could remain negatively buoyant. The addition of this energy path to PLM89A seems relatively easy, however, it would certainly place the chemistry in PLM89A as the most complete description.

The use of a finite-rate reaction scheme in PLM89A is significant because the alternative models do not currently possess this feature. Examining the value of a finite-rate scheme in the UF_6 application is therefore worthwhile since use of a model other than PLM89A will require significant enhancement to include such a scheme. The reactions of interest for the safety analysis application are generally very fast, so a cursory inspection might suggest that the steady-state approach of ADAM/HGSYSTEM and Rodean (1991) would be sufficient. However, chemical reaction between two species requires that they be mixed at the molecular level. The mixing between UF_6 and water, for example, occurs as water is entrained into the gas cloud from the surrounding atmosphere. This process is effected by turbulent eddies, which mix the two components on a length scale comparable with the scale of the entraining eddies themselves. The turbulent cascade process continues to mix on smaller and smaller scales until the species are thoroughly intermingled, but the initial reaction occurs only at the interface of the cloud. The interface is highly distorted by the turbulent eddies, but the thorough mixing takes a finite time to accomplish. Thus, even though the reaction may be very fast, the rate of reaction can be controlled by the ability of the turbulence to mix the two components. The importance of this process has been discussed by Donaldson and Hilst (1972), and modeled numerically by Riley et al. (1986) for a mixing layer and by Sykes and Henn (1992) for a reacting plume in a turbulent boundary layer.

PLM89A contains a parameterization of the turbulent mixing effects, and reduces the rate of reaction as appropriate for the turbulent time scales of the cloud. The improvement of reactive plume models is a current research topic for the atmospheric dispersion community, and several approaches are possible. The two major options are use of "instantaneous" plume spread rates, and parameterization of the fluctuation correlations associated with the turbulent diffusion process. PLM89A uses an empirical estimate for the species correlation, but it should be noted that there is very limited experimental support for the estimate. The alternative use of "instantaneous" spread rates is based on the assumption that the instantaneous plume is well-mixed, and that neglect of the large-scale meandering component is sufficient for estimating chemical reaction rates. This assumption may be reasonable at short downstream distances, where the meandering effect is clearly visible, but becomes less reliable further downstream. Both approaches give a reduced reaction rate and at present there is no particular reason to prefer one method over the other. In practical terms,

the use of instantaneous spread rates is more readily adapted for use with models like HGSYSTEM and ADAM.

The nonuniformity of the mixing process may lead to significant dynamic effects in the case of an exothermic reaction. The concept of a separated cloud is a likely product of the confinement of the reaction to the plume edges. Since the reaction proceeds quickly, the heat is released at the upper surface of a ground-hovering plume where water is brought into contact with the cloud reactants. Thus, instead of uniformly heating the entire cloud, a tenuous cloud of hot gas would rise from the surface as it reacted, leaving the bulk of the cloud as a dense, unreacted layer on the ground. Incorporation of this effect into the safety analysis model would clearly require modification of the Gaussian distribution assumption, and will be discussed further in the next section.

3.6 Turbulent Chemistry Leading to Plume Separation

The details of the chemical reaction between the UF_6 in the cloud and the ambient water (vapor or droplets) are dependent on the turbulent mixing, but are not well understood. As discussed above (Section 3.5), the reactions are localized in the region of the interface; and this localization of the heat release from the reaction could have significant dynamic consequences. It is important that the safety analysis model contain the capability to describe these effects, but the uncertainty in our current understanding implies that the model should be run in a "bounding" mode, with reasonably extreme assumptions employed to determine the range of possibilities. One of these extremes is clearly the "perfect mixing" assumption used in ADAM and HGSYSTEM, and easily implemented in PLM89A. A different assumption is that the speed of the reaction is limited by the turbulent mixing, which requires some effort to model in ADAM and HGSYSTEM. In this mixing-limited mode however there is still some uncertainty in the spatial distribution of the exothermic heat release. The extreme assumptions here would be that the heat is released uniformly throughout the cloud, or that the heat is released in a thin shell on the cloud boundary. In summary there are three possible cases, as illustrated in Fig. 3.2:

1. Perfect mixing — complete reaction and uniform heat release,

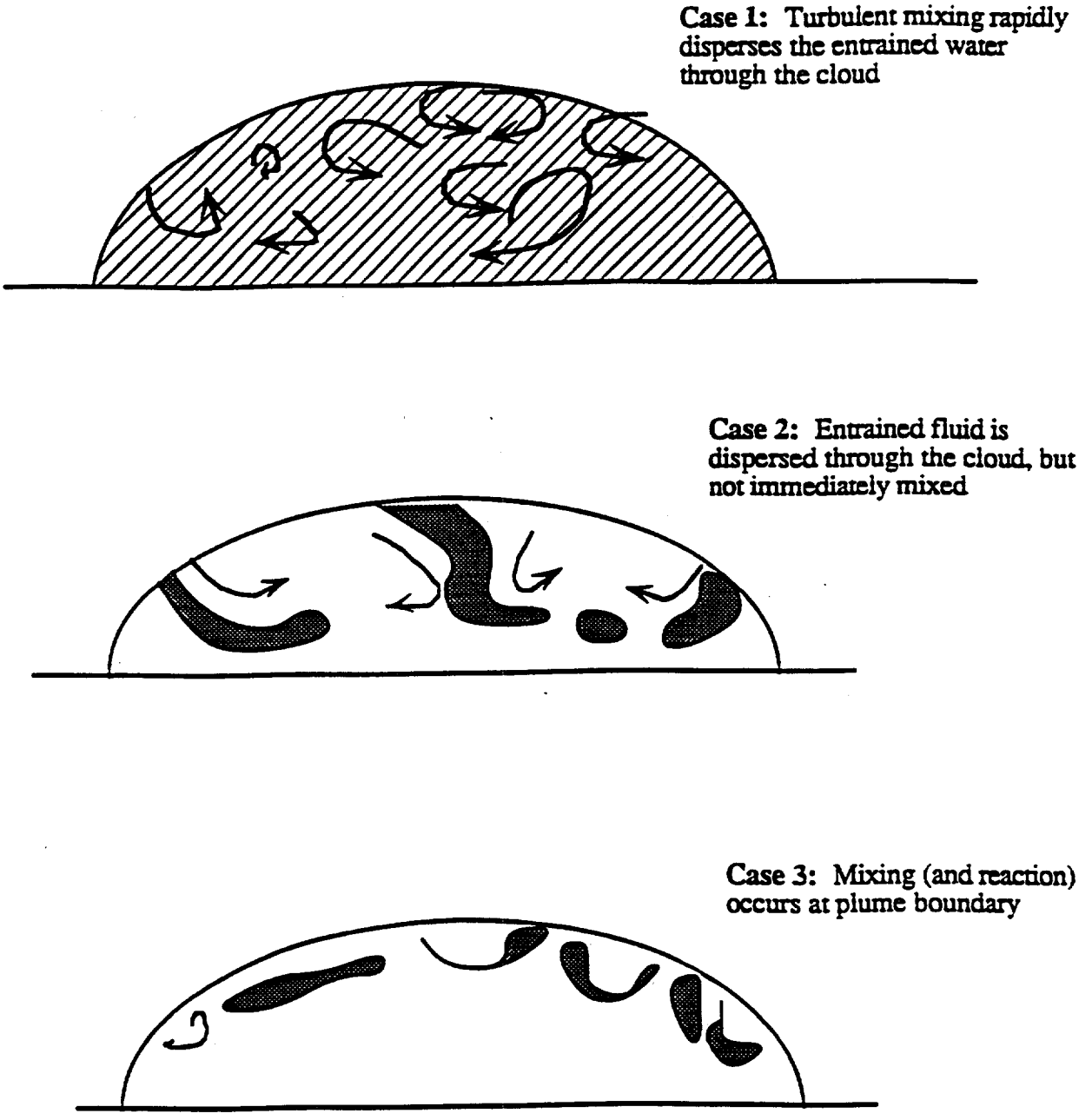


Fig. 3.2. Schematic of different mixing assumptions for the cloud.

2. Incomplete mixing with uniform heat release, and
3. Incomplete mixing with localized heat release.

We proceed to discuss how these three cases could be modeled using the candidate frameworks. There are only two frameworks under consideration, namely PLM89A and that of ADAM/HGSYSTEM.

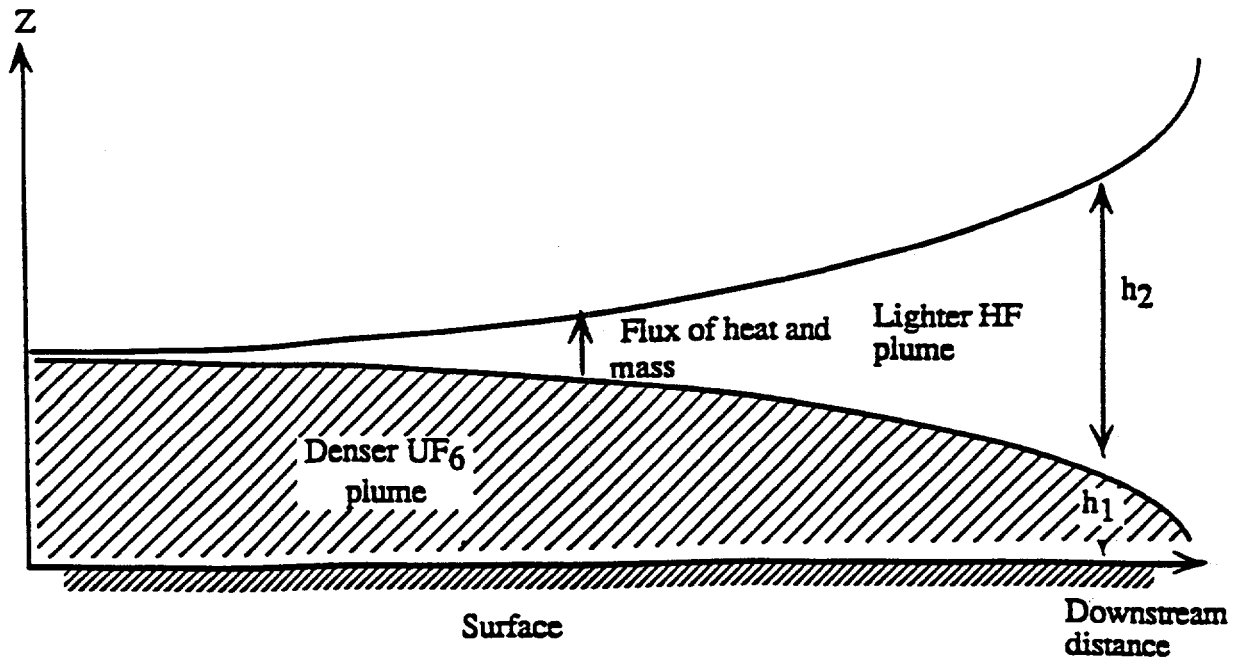
3.6.1 PLM89A

Case 2 is the default mode of operation for PLM89A, so no modifications are required for this case. Case 1 can also be optionally implemented, although this does introduce timestep restrictions on PLM89A, since the model timestep is already controlled by the chemical reaction rates. An implicit steady-state scheme similar to that of Rodean (1991) is also available as an option within PLM89A.

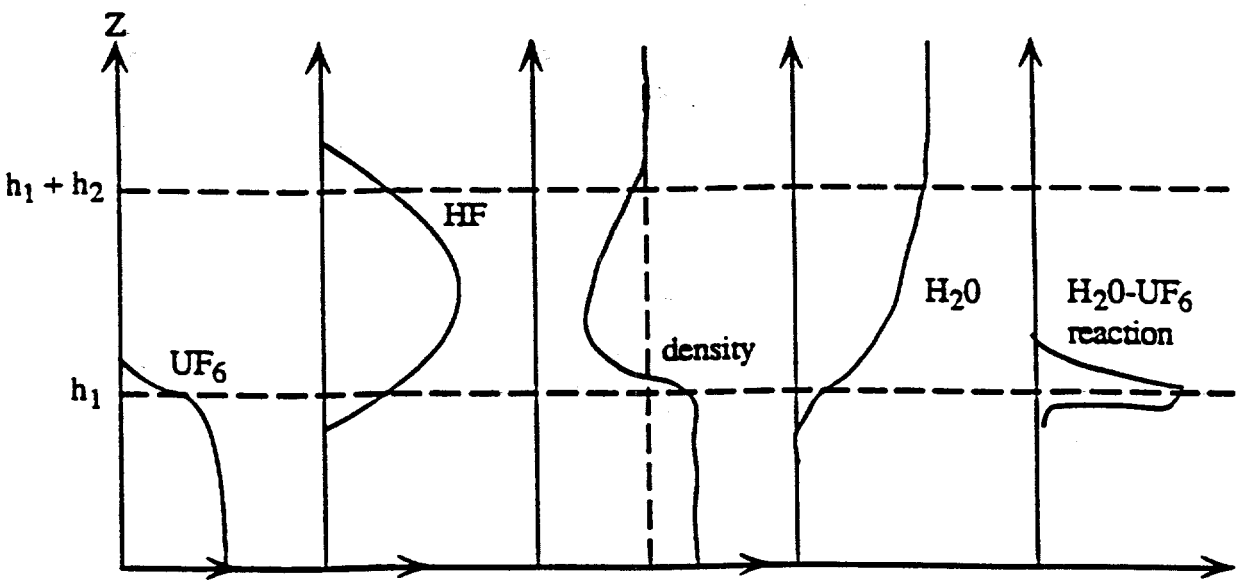
The third case to consider is more complicated since it involves a change in the dynamics of the cloud. The assumptions in this case lead to a "separated" plume, as the localized heat release warms a thin layer of gas which can then move vertically and leave the main cloud as its buoyancy becomes positive. This has to be tracked as a separate plume and consequently requires significant code modification.

There are two possible ways to incorporate these effects into PLM89A. One could compute two separate plumes simultaneously, or save an effective plume source from the initial computation and run a second plume calculation to model the separated phase. The essence of the model is a transfer of mass between the two plumes, as illustrated schematically in Fig. 3.3(a). The profiles of plume concentrations and density are shown schematically in Fig. 3.3(b). At each timestep, the mass of HF produced by the water-UF_6 reaction, along with the heat energy produced in this reaction, is transferred from the ground-hovering plume into the separated plume. Thus, using the current definition of the reaction rate from PLM89A, the mass of the entrained water that reacts with UF_6 in a timestep is m_w, for example, where

$$m_w = \text{Reaction rate} \times \text{Concentration of } UF_6 \times \text{Mass of water} \times \text{Timestep}.$$



(a) Schematic illustration of the two plumes



(b) Schematic illustration of typical separated plume profiles

Fig. 3.3. Illustration of the separated plume geometry.

If the reaction is fast enough to use all the entrained mass, then the latter would impose a limit on the reaction. Similarly, if the supply of UF_6 is the limiting factor, this would provide the limit. In general, however, we are assuming that the supply of both reactants is adequate and that the reaction is limited by the turbulent mixing process. We assume that the mass, m_w, of water reacts with mass, m_{UF6}, of UF_6 to produce a mass, m_{HF}, of HF, releasing heat energy, J. If the ambient water-air mixing ratio is q, say, and the mass mixing ration of UF_6 in the plume is c_{UF6}, then the reacted volume will contain a mass, m_{HF}, of HF and mass, $(m_w/q + m_{UF6}/c_{UF6})$, of air. The plume concentrations should strictly vary as a Gaussian function across the plume, but a simple estimate of the reacting concentration can be taken to be 50% of the centerline value. The reacted volume is transferred from the lower plume to the upper, reducing the mass of UF_6 in the lower plume by an amount, m_{UF6}; all other constituents of the reaction volume are similarly transferred into the upper plume. The entrained water-air mixture is therefore not added to the lower plume, since it has reacted to produce HF and heat and immediately becomes part of the upper plume.

The vertical spreads of the two plumes are changed by the transfer so that the mass concentration of UF_6 in the lower plume and HF in the upper plume are unchanged (i.e., the changes in volume resulting from the transfer must be accounted for). Thus, if a fraction, f, of the total UF_6 is consumed in the reaction during one timestep, then the vertical spread of the lower plume is also reduced by this fraction. The spread of the upper plume is also increased by the amount lost from the lower plume plus the effective entrainment depth over the timestep. The upper plume therefore receives a continuous input of HF and heat, while the lower plume loses UF_6 but remains dense. This modeling concept relies on a somewhat simplified view of the chemistry of the plume, and will therefore need to be considered by more qualified personnel from the point of view of the reaction system. Some account of the shielding due to the upper plume could also be included by basing part of the entrainment on the upper plume constituents rather than ambient values. In order to maintain a relatively simple description, one could assume that the horizontal distributions of the two plumes are the same (i.e., the lower plume determines the lateral structure since it acts as the source for the upper plume). This model neglects the effect of entrainment at the lateral boundaries on the reaction, effectively assuming that the plume is shallow and wide, but a more detailed treatment would require a fully resolved spatial distribution which is difficult to justify in light of the uncertainties in the turbulent reaction mechanisms.

It is clear that even the simplified representation just outlined is a difficult undertaking, and will require significant development and testing. The need for this development depends on the importance of the exothermic heating, so investigations should be made to determine whether the localization is important. Detailed three-dimensional simulations could possibly be used to examine the flow structure and assess the assumptions of the two-plume model described above. If the heating can be neglected entirely, presumably a conservative assumption from the point of view of ground-level concentrations, then the separated plume phenomenon can be avoided.

3.6.2 ADAM/HGSYSTEM

Case 1 is the standard mode of operation for these models, so no modification beyond the implementation of a UF_6 reaction scheme would be required. Case 2 would be effectively implemented by only allowing a fraction of the entrained water to be passed to the chemistry subroutine (i.e., only the fraction entrained into the instantaneous plume would be considered as available for reaction). This could be determined using a similar turbulence timescale limit on the reaction to that in PLM89A, so that the mass involved in the reaction would be defined as a part of the entrained mass, exactly as shown in the previous section for the exothermic transfer between the two plumes for Case 3.

Case 3 involves a similar level of complexity for ADAM and HGSYSTEM as it does for PLM89A, since we are forced to model two separate clouds. A similar scheme could be used, with transfer of mass and heat from a dense, lower UF_6 plume into a hot, upper HF plume. ADAM and HGSYSTEM provide the capability for modeling interaction with the ground and continuous sources, although they would obviously require significant modification .

3.7 Effects of Statistical Fluctuations

Atmospheric dispersion has an inherent random component, induced by the large range of length scales involved. An apparent randomness is evident to even the casual observer of real plumes or puffs dispersing in the atmosphere. The instantaneous contours of constant concentration are quite distorted, in sharp contrast to the smooth contours assumed in the Gaussian models. The Gaussian distribution is approached when a large number of observations are averaged to obtain an ensemble mean. In spite of the widespread recognition of the existence of this random component

of atmospheric dispersion, all of the candidate models considered here only model the ensemble mean evolution of the plume. This is a direct result of the fact that the input winds and dispersion are given in terms of some average, mean conditions. None of these models attempt to incorporate any contribution of the random departures from the mean. We believe this is a serious deficiency, which will not be easy to rectify.

The difference between the mean and individual sample concentrations taken with a fast response sampler can be orders of magnitude. This leads to the evaluation difficulties discussed in Section 2.2 when one is interested in peak concentrations obtained over short-time intervals. The nearest one can come with a deterministic prediction of the concentration is to eliminate the effects of meander on dispersion and restrict the plume spread to only the minimum possible in the available sampling time. Then this maximum concentration as a function of travel distance may be compared with the observed maximum as a function of travel distance without regard to the angular position at which the maximum occurs. This requires that the sampling network be sufficiently dense that it indeed samples the maximum concentration.

Three of the candidate models do incorporate the feature of adjusting the plume spread for short sampling times, i.e., PLM89A, SLAB and HGSYSTEM. They reduce the horizontal spread by a factor of

$$(T_{sample}/15\ \text{min})^{0.2}$$

where T_{sample} is the sampling time, following Slade (1968). This reduction in plume width for short sample times is based on estimates of the lateral velocity fluctuation spectrum, and is only valid for finite duration sampling of a meandering point source. Neither TRIAD, nor ADAM currently include this feature. A rough estimate of the probabilities associated with the statistical plume fluctuations may be incorporated by computing two separate spread rates for the plume; one for very short sampling times to obtain an "instantaneous" plume spread, and a second spread for the maximum time interval of interest. Probabilities may then be estimated using the Gifford (1959) meandering plume model. For this to have much credibility, it would be necessary to replace Slade's empirical power law reduction factor with a rational computation of the instantaneous plume scale based on the concepts of relative diffusion. The current practice of assuming an arbitrary short sampling time (e.g., 19 s for HGSYSTEM) to represent instantaneous concentrations is inadequate

for the UF_6 safety analysis, because it simply reduces the spread by about a factor of 2 from the standard prediction. This factor applies at all distances and for all sources under all conditions, and therefore cannot account for the effects of source size and turbulence length scales, which are known to be important.

3.8 Source Modeling

The source modeling of the initial introduction of the UF_6 into the atmosphere is an essential phase of the proposed safety analysis. The same mass released from a small vent on the roof with momentum and buoyancy, may present a different hazard than if it is released as a flashing liquid. This source modeling must either be contained within the model or some pre-processing is required before the model is run. PLM89A has some capabilities for dealing with different type sources, primarily as a pre-processor calculation. HGSYSTEM contains a number of pre-processing modules for representing different release scenarios. ADAM also represents several types of accidental release, including pressurized jets and evaporating pools, and will compute the release parameters from user specification of the fracture dimension and storage mass and pressure. SLAB provides for jet and pool releases but the release parameters must be computed before initializing SLAB. TRIAD can only model a buoyant jet release, and requires input of the source size and fluxes.

One of the most complex issues involved in the source modeling for a UF_6 release is determining the proper partitioning between the solid and vapor phases. Many of the creditable releases involve high pressure liquid, which flashes into a combination of solid particles and vapor when exposed to atmospheric pressure. The subsequent dispersion of these particles is critically dependent on their physical size. PLM89A assumes an implicit particle size based on small scale laboratory experiments. This is likely to remain a significant source of uncertainty in the model output.

3.9 Model Evaluation Status

Three of our candidate models have been included in the evaluation study of Hanna et al., 1991; SLAB directly and TRIAD and HGSYSTEM, indirectly represented by their respective dispersion modules, INPUFF and HEGADAS. In their summary, both HEGADAS and SLAB qualify as one of the six models given the rating of "better" models. They conclude that "the better

models can have their predictions within a factor of two of the observations about 70 - 80% of the time". INPUFF did well on the passive releases, but poorly on the dense gas releases. As stated in Section 2.2, we believe this evaluation implies a higher performance than should generally be expected from the models.

In an independent evaluation study involving a smaller number of models (including only SLAB from our candidate list) and three data sets, Touma et al., 1991 found that SLAB predictions agreed with maximum concentrations within a factor of 2 for one of the data sets, but consistently underpredicted by a factor of 2.5 - 3 for the other 2 data sets. They note that the initial characterization of the source release is critical; that models which contain similar treatment of atmospheric dispersion and utilize the same meteorological inputs predict concentrations which differ by more than an order of magnitude.

PLM89A has undergone a number of internal checks, and was the subject of the earlier review by Hicks et al., 1985. In that review there was some indication that plume rise was underpredicted for steady-state, non-reactive constituents (Campbell et al., 1985), but the general conclusion was that it behaved reasonably well under the conditions for which it was designed. Its major defect was the absence of a number of features to be discussed in Section 4.1. PLM89A has been used to analyze actual releases of UF_6. Good agreement, within a factor of 5, is claimed based on comparisons between maximum measured and maximum predicted uranium and fluoride concentrations.

3.10 Acceptance Status

Based on their greater number of "successful" evaluations SLAB and HEGADAS may be expected to enjoy a wider acceptance than either PLM89A or TRIAD for short range vapor cloud dispersion. Since HGSYSTEM uses the HEGADAS dense gas dispersion routines, it shares this acceptance. ADAM has also been evaluated against several of the standard data sets, with comparable results to the other dense gas models. For longer ranges out beyond several kilometers, TRIAD may be expected to be more generally accepted, since it uses the standard EPA model INPUFF. However, since any of these models must be significantly modified to

obtain the desired safety analysis model, the acceptance of the "new" model should be expected to be based on demonstrations of new evaluation comparisons.

4. POSSIBLE ROUTES TO THE SAFETY ANALYSIS MODEL

4.1 Starting From PLM89A

As discussed in the previous section, a number of deficiencies in PLM89A would need to be corrected before its implementation as the safety analysis model. The major advantages of PLM89A are its sophisticated description of the UF_6 chemistry and the fact that its status as an "in-house" code makes development easier than changing an unfamiliar code. We must determine the extent of the required modifications, however, to decide the feasibility of using PLM89A as the model basis.

The major improvements we see as necessary for PLM89A area)

1. transient dynamics,
2. improved dense gas dispersion,
3. improved atmospheric dispersion,
4. building/terrain effects,
5. incorporation of latent heat of evaporation for water droplets, and
6. at least a rough estimate of statistical fluctuations.

Transient dynamics were discussed in Section 3.3, where it was suggested that PLM89A could be upgraded relatively easily to give a reasonable description of a transient release. The extension of the transient "window function" to the calculation of the nonlinear processes would place PLM89A at the same level of sophistication as the other candidate models.

Dense-gas dispersion is the major distinguishing feature for PLM89A, since there has been considerable research and development of models for this phenomenon. The description in PLM89A is restricted to the gravitational spreading effect of a dense cloud in contact with the ground. The spread velocity parameterization is similar to the current dense gas models, but PLM89A does not model the diminished vertical entrainment due to the stable density gradient. This could be remedied

by incorporating the entrainment formula from one of the accepted dense-gas models. SLAB uses a very complicated description, which appears to be more general than the other models. ADAM and HEGADAS use simpler formulations which should be readily adaptable for use in PLM89A. However, it must be recognized that implementation of a sub-model from one of the dense gas models, even a relatively simple parameterization, does not imply that all the dense gas evaluation results associated with the sub-model are valid for the enhanced PLM89A. The model evaluations have been performed for the complete model system, so some re-testing of the new model would be required to demonstrate that the sub-model works the same way.

The representation of dispersion due to ambient atmospheric turbulence is arguably close to satisfactory in PLM89A. From our own perspective, the use of empirical PGT stability categories does not properly describe the turbulence structure of the planetary boundary layer. For any particular occasion, the turbulence depends on the wind speed, the surface heat flux, surface roughness, mixed layer depth, and perhaps other parameters. It cannot be described adequately by means of a wind speed and a stability category. However, the use of the PGT scheme is still widely accepted for regulatory purposes and it can be argued that the range of diffusion rates covered by the PGT categories provides a plausible representation of the short range dispersion for a surface release. We do not believe that the PGT predictions of horizontal dispersion are reliable for the instantaneous concentration values of importance to the chemical reactions. The prediction from the PGT scheme would not be reliable for emergency response applications either, where the particular atmospheric conditions are important. Physically-based turbulent dispersion estimates are available and could be implemented in PLM89A, but they have not been as widely applied and tested as the PGT method.

We have outlined a procedure in Section 3.1.5 for incorporating the PGT stability classification system within a turbulence-based dispersion representation. This procedure requires some development of specific parameterizations, but would replace the current use of an effective origin for the empirical power law spread curves with an ambient entrainment velocity based on a consistent boundary layer profile specification. The vertical entrainment rate should be modified by the stability dependent formula adopted for the dense ground-hovering cloud, and will give a smooth transition to the passive dispersion phase at late time.

The implementation of building effects in PLM89A is probably as difficult, or as easy, as it is for any of the other candidate models. None of the models contain any specific description of these effects, and we do not believe any sophisticated scheme can be justified. An increased surface roughness for the plant area is appropriate for representing the enhanced turbulence levels around the buildings, and a limit on the lateral spread can be imposed to represent the "channeling" of clouds between buildings.

The enhancement of the thermodynamic model in PLM89A to include latent heat of vaporization of water for fog situations does not appear to pose any significant difficulty.

A rough estimate of the probabilities associated with the statistical plume fluctuations may be incorporated by computing two separate spread rates for the plume; one for the instantaneous plume, and a second for the maximum time interval of interest. Probabilities may then be estimated using the Gifford (1959) meandering plume model.

The features of this upgraded version of PLM89A, which we will temporarily call PLM92, may be compared with the desirable features of a revised model given by Hicks et al., 1985. Let us briefly consider each of the 8 factors they listed:

1. A puff model is recommended so that it can handle light winds and short-term releases. The incorporation of the window function to approximate transient dynamical effects, should allow PLM92 to simulate light wind, short-term releases as well as most puff models.

2. Initial dilution should be handled using site-specific parameterizations.

3. A consistent puff rise formulation needs to be developed. The incorporation of the window function to approximate transient dynamical effects, should provide a reasonably consistent puff rise formulation for PLM92. It at least will permit it to simulate buoyant puff rise much more consistently than INPUFF used by TRIAD.

4. Dispersion calculations should make use of direct turbulence measurements or modern scaling relationships, rather than the Pasquill/Gifford categories. This feature is not included in the modifications outlined above. This is less important if PLM92 is not to be used as an emergency response model.

5. Transport needs to be addressed, to account for terrain-induced effects (three-dimensional, and site specific). This is not included but again seems less important as long as PLM92 is not to be used as an emergency response model.

6. A capacity to accept real-time data is desirable, to make the model suitable for real-time emergency response applications. Response is the same as that to items 4 and 5.

7. Atmospheric variability should be addressed by incorporating a model capability to estimate variances and peak-to mean ratios. The outlined modifications do provide a way for roughly including this effect.

8. Tests of model components should be conducted, using field, laboratory, and theoretical methods. We believe this should be an important part of the new model development, regardless of the route taken to achieve it. It will discussed further in Section 5.3.

4.2 Starting From TRIAD

Amongst our candidate models, TRIAD probably requires the most extensive development before it would meet all the requirements of a safety analysis model, and is therefore not considered an optimum basis for the safety analysis model. Williams (1989) has noted the deficiencies of this model for the UF_6 safety analysis. It appears that only two of the concerns raised by the earlier review (Hicks et al., 1985) of PLM89A have been improved by TRIAD; it has an improved capability to handle light variable winds, and site specific turbulent data. Two major problems, where it is more deficient than PLM89A, are its lack of any description of dense gas effects and its dependence on simple correlations for its chemistry. It shares the rest of the uncertainties of PLM89A on a more or less equal basis. It appears that the bulk of the effort in the development of TRIAD was directed toward a treatment of a time-dependent and spatially varying wind field so it could also be used for an emergency response model. The use of a puff model has driven the developers toward a very

simple representation of all the dynamic effects and chemical reactions, so that they are all included as initial conditions for a puff. Thus, all the plume rise and chemical transformation occurs within the first time step for a puff, and the subsequent evolution is determined by the ambient conditions. A proper representation of dense gas effects within the TRIAD framework would be a significant effort. The model would need to take small timesteps and consider the interaction between overlapping puffs. The small time step would also necessitate a more sophisticated treatment of the UF_6 chemistry so that it could interact with the dynamics in a more consistent manner.

Starting from TRIAD would appear more favorable if the desired model was also to be used as an emergency response model, since TRIAD is the only one of the models considered in Section 4 which allows for the input of general 4-D (space and time) winds. An attractive emergency response model could be developed by using the new safety analysis model as an effective source module representing the dispersion out to approximately 1 km, and using TRIAD for dispersion beyond 1 km, with the 4-D wind field input from on-site measurements. Since most of the dense gas effects and chemically induced dynamics should be restricted to within 1 km, and most of the local site wind steering may be expected to occur beyond this range, TRIAD could provide the basis for a feasible emergency response model. As noted by Williams (1989), its extensive input requirements would need to be simplified. We believe there should also be an automated link between the on-site measurements and the computer model to make such an emergency response tool attractive. However, such a combined model would still lack a comprehensive treatment of fluctuation statistics which we consider to be an important feature.

4.3 Starting From HGSYSTEM

HGSYSTEM embodies the dense gas module of HEGADAS with a description of HF chemistry with polymerization effects, which is very relevant for the UF_6 safety application. Hydrogen fluoride is one of the major products of the reaction between UF_6 and water, so the inclusion of HF chemistry is a very useful feature in the dispersion model. HGSYSTEM contains several sub-modules to describe a range of source effects, including jets and evaporating pools. It basically simulates a continuous release, and only has limited capability for simulating transient releases. HGSYSTEM has been evaluated against a number of dense gas data sets and HF test releases, providing relatively good credentials for the code.

The deficiencies of HGSYSTEM for the UF_6 safety analysis application are:

1. UF_6 chemistry,
2. improvements to PGT turbulent dispersion,
3. instantaneous release dynamics,
4. building/terrain effects, and
5. concentration fluctuations.

The extension of the chemistry description to include the UF_6 reactions and other uranium species may not be an easy task. The simplest approach would be to implement Rodean's (1991) scheme, or an equivalent simplification of the PLM89A chemistry. The current description of chemical reaction in HGSYSTEM uses assumptions of fast reaction and perfect mixing to determine the chemical composition and thermodynamics of the gas cloud, but this is not justified for the mean UF_6 plume. However, it should be a reasonable approximation for the instantaneous plume, if the plume width algorithms are changed to properly represent the instantaneous plume. Modifying the codes to represent uniform mixing, fast reaction within the instantaneous plume should be roughly equivalent to the finite-rate chemistry, with a turbulence-limited reaction such as modeled in PLM89A. The problem of representing the confinement of the exothermic reaction to the plume boundary is essentially the same regardless of which model one chooses to start from. The effect of this localization is to produce a heated layer that can detach from the dense cloud, and the representation of this phenomenon is a difficulty for any Gaussian-type model.

HGSYSTEM uses the PGT representation of the ambient atmospheric diffusion in a similar way to PLM89A. The effort required to upgrade this method along the lines of Section 3.1.5 is probably very similar to upgrading PLM89A. Both models currently use an entrainment velocity concept to spread the plume in response to the dynamic effects of jets and gravitational spreading, so the augmentation of this entrainment by an ambient value dependent on plume altitude and meteorological conditions should not be difficult. The extension of the dispersion scheme would naturally provide a description of the sampling-time dependence of the concentration values and thus address the fluctuation issue.

HGSYSTEM does not provide for a transient buoyant source. It may prove reasonably conservative to ignore this effect for the safety analysis, in which case HGSYSTEM would not need

modification. However, if it is required then the mode would need to be extended to include some account of three-dimensional dispersion in the transient rise phase, using the "window" function for the dynamic variables as suggested for PLM89A. We are already recommending that the atmospheric turbulence representation be extended for the safety analysis, so the current limitation to the surface layer would be removed.

Building/terrain effects are currently absent from HGSYSTEM but the simple model of building channeling would be a minor modification. HGSYSTEM does currently have the ability to represent changes in roughness, so some of the effects are already included.

4.4 Starting From ADAM

ADAM is very similar in capability to HGSYSTEM. It has a similar set of dense gas effects parameterizations, although they are different in detail, and like HGSYSTEM, ADAM contains a description of HF chemistry. ADAM provides a slightly more general framework for the inclusion of new chemistry, since it already describes a number of different reaction systems. ADAM can simulate jet and evaporating pool releases, and can also treat continuous and instantaneous releases. It uses the PGT diffusion rates to represent the ambient atmospheric effects. The model has been evaluated against a number of dense gas data sets with reasonable success.

The deficiencies of ADAM for the UF_6 safety analysis application are identical to those of HGSYSTEM, i.e.:

1. UF_6 chemistry,
2. improvements to PGT turbulent dispersion,
3. instantaneous release dynamics,
4. building/terrain effects,
5. concentration fluctuations, and
6. transition to positive buoyancy and plume lift-off, if required.

ADAM does not provide for a transient buoyant source or for transition to positive buoyancy in the cloud. It may prove reasonably conservative to ignore these effects for the safety analysis, in which case ADAM would not need modification. However, if they are required, then the entrainment rates would need to be extended to account for positive buoyancy, and to include some

account of three-dimensional dispersion in the transient rise phase, using the "window" function for the dynamic variables as suggested for PLM89A. We are already recommending that the atmospheric turbulence representation be extended for the safety analysis, so the current limitation to the surface layer would be removed.

The effort required to modify ADAM to meet the safety analysis requirements is presumably the same as that for HGSYSTEM.

4.5 Starting From SLAB

Lawrence Livermore's SLAB model (Ermak, 1990) would require similar modifications to those required for HGSYSTEM and ADAM. SLAB has a more complicated dense gas formulation, as discussed in Section 3.2.2, and does go part of the way toward our concept of a turbulence-based dispersion scheme. SLAB already assigns values of the Monin-Obhukhov length to PGT stability classes, and prescribes a full profile of the mean wind and turbulent entrainment velocities throughout the depth of the turbulent boundary layer. The shape of these profiles is not fully consistent with our understanding of boundary layer dynamics, however, and the treatment of time-averaging effects is also based on over-simplified assumptions. The details of the parameterizations would therefore need to be changed, although the framework for most of the changes does exist within SLAB.

Other effects such as building channeling and transient buoyant sources would need to be included in SLAB.

We believe that the increased generality of the turbulent entrainment parameterization in SLAB does not balance the need to incorporate the exothermic chemistry. It seems considerably easier to modify the dispersion parameterizations within the other codes than to include the complex chemical reaction systems in SLAB.

5. RECOMMENDATIONS

5.1 Tradeoffs Involved in Making the Model Development Paths

A specific recommendation of the best development path requires more information than we currently have. What we can do is to say how additional assumptions would decide the development path. This allows the readers to use their own judgement as to the validity of the particular assumptions, and thus arrive at their judgement as to which development path would be best.

If we assume that Energy Systems intends to do the necessary code modifications in-house, and thus that their familiarity with PLM89A should make it much easier for them to modify, than it would be for them to modify HGSYSTEM, or one of the other two dense gas models considered here, then the best path is likely to involve using PLM89A to develop a substantially modified PLM92 as outlined in Section 4.1. However, this apparent advantage may be nullified by the fact that HGSYSTEM is a newer code developed for wider use, and thus may be sufficiently modular to permit easy modifications. If this is the case, which could only be determined by analyzing the two codes, the best choice may be to start from HGSYSTEM and develop an expanded model with UF_6 capabilities which might be termed UHS via the route outlined in Section 4.3. We are transmitting a copy of the source code for HGSYSTEM along with this report to allow the appropriate modelers at Energy Systems to re-evaluate this assumption.

Our basis for favoring HGSYSTEM over SLAB or ADAM, is not overly compelling. We assume that it should be advantageous to start with a system that models the HF chemistry, and add UF_6, than it is to start with no chemistry. This assumption puts HGSYSTEM and ADAM ahead of SLAB. HGSYSTEM is then favored over ADAM because of its more modular construction, and because its main module, HEGADAS, has enjoyed wider testing as a dense gas model than has ADAM.

If we make the opposite assumption, that the combined UF_6 and HF chemistry is sufficiently coupled that there is no great advantage to starting with a model with its own version of HF chemistry, then the optimum path may be to start with SLAB and develop an expanded model with UF_6 capabilities which might be termed USLAB via the route outlined in Section 4.5. This path

could take advantage of SLAB's description of atmospheric diffusion which is somewhat closer to the method proposed in Section 3.1.5.

Another important assumption is that the newly revised model will be exposed to fairly extensive new evaluation exercises as recommended in the next section. If time and resources do not permit this, then it may be a little easier to get acceptance of either UHS or USLAB model results than it would be to get acceptance of PLM92 results, based on the wider testing that HEGADAS and SLAB have enjoyed. We are not saying that these two models are likely to produce more reliable results, only that they are likely to be more readily accepted.

Finally, we note that if we change the low priority for using the newly revised model as an emergency response model (i.e., if the requirement for such a capability were to exist) then the best path to attainment of such a model may be by adding on a version of TRIAD for distances beyond 1 km as outlined in Section 4.2. This priority could also slightly favor ADAM for the short-range model basis due to its wider data base of chemical reactions.

5.2 Recommended Evaluation of Newly Modified Model

Any of the paths chosen under 5.1 will involve a number of detailed code changes to the respective parent model. The revised model should be extensively tested to check that the programming is done correctly and that the desired effects are now indeed incorporated. This is likely to involve a significant fraction of the time allotted to modify the model.

The model should be given both theoretical tests and comparisons with real data. The first may be done by exercising the model for a number of different scenarios and checking that it behaves in a reasonable manner and satisfies a number of theoretical consistency checks. Hanna and Strimaitis (1989) provide a workbook of test cases for vapor cloud source dispersion models. They consider 5 different source scenarios including elevated dense gas jets, horizontal two-phase jets, valve choked flow, liquid spills on the surface. Although the particular different chemical species involved in these scenarios are not appropriate for the new model, this does represent a minimum set of source conditions for which the UF_6 model should obtain reasonable results.

Consistent comparisons with real data are more difficult. The limited data available on actual releases of UF_6 does not seem adequate to instill confidence in the model. In fact, the comparisons made with results from PLM89A, already pass these tests. Ermak et al., 1988 has put together a summary of 26 field tests of dense gas dispersion. The intent is to provide sufficiently complete data for anyone to run and evaluate their model. A brief outline of the characteristics of the subset of these chosen by Hanna et al., 1991 for their evaluation tests are given in Table 5.1. Comparisons with some of these same cases would allow the new model performance to be compared with the performance of some of the models considered in Section 2.

The incorporation of the appropriate chemistry and dispersion representations into one of the candidate models will provide a reasonably complete description of UF_6 dispersion for use in the safety analysis. The level of uncertainty in the predictions of the final model should not be underestimated, however. While the principal physical processes will be represented in the best available manner within the context of a simplified model, the uncertainties in the predictions are likely to be larger than the currently reported discrepancies between dense gas measurements and predictions. We would only expect the model to correctly estimate the results of anticipated scenarios to within an order of magnitude. Any significant reduction in this order of magnitude uncertainty must be established by careful comparisons between field tests and model simulations.

Table 5.1. Summary of characteristics of datasets as given by Hanna et al., 1991

	Burro	Coyote	Desert	Goldfish	Hanford Kr^{85}	Hanford Kr^{85}	Maplin	Prairie	Thorney Island	Thorney Island
Number of Trials	8	3	4	3	5	6	4.8	44	9	2
Materials	LMG	LNG	NH_3	HF	K^{85}	K^{85}	LNG,LPG	SO_2	Freon & N_2	Freon & N_2
Type of Release	Boiling Liquid	Boiling Liquid	2-Phase Jet	2-Phase Jet	Gas	Gas	Boiling Liquid	Gas Jet	Gas	Gas
Total Mass (kg)	107000-17300	6500-12700	10000-36800	3500-3800	11024[a]	10[a]	LNG:2000-6000 LPG:100-380	23-63	3150-8700	4600
Duration (s)	79-190	65-98	126-381	125-360	598-1191	(Instantaneous)	60-360	600	(Instantaneous)	460
Surface	Water	Water	Soil	Soil	Soil	Soil	Water	Soil	Soil	Soil
Roughness	0.0002	0.0002	0.003	0.003	0.03	0.03	0.0003	0.006	0.005-0.018	0.01
Stability Class	C-E	C-D	D-E	D	C-E	C-F	D	A-F	D-F	E-F
Max. Distance (m)	140-800	300-400	800[b]	3000	800	800	400-650	800	500-580	472
Min. Averaging Times (s)	1	1	1	66.6-88.3	38.4	4.8	3	(Dosage)	0.06	30
Averaging Time (s)	40-140	50-90	80-300	66.6-8.3	270-845	4.8	3	600	0.06	30
Qualitative Assessment:										
Lateral Resolution	Good	Good	Good	Good	Good	Good	Marginal	Good	Good	Good
Temporal Resolution	Good	Good	Good	Fair	Good	Good	Good	Fair	Good	Good

[a]Curies rather than kilograms are used as a measure of the amount of this radioactive tracer released.

[b]Concentrations are measured beyond 800 m, but these are not well-instrumented measurement arcs.

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APPENDIX

Implementation of an Advanced Turbulent Dispersion Scheme

In this appendix, a more complete description of the turbulence-based dispersion scheme recommended in Section 3.1.5 is presented. The specifications for the velocity and turbulence profiles are given for a range of atmospheric conditions, and the relation with the PGT stability classes is examined.

The turbulence generated by surface layer processes (i.e., shear production and buoyancy generation, can be represented in terms of standard boundary layer parameters). These are wind speed (U), surface heat flux (H_0), surface roughness length (z_0), and mixed layer depth (z_i). Other factors may modify the boundary layer structure, such as transient effects, thermal wind shear, or terrain influences, but the normal equilibrium conditions can be described reasonably well with the standard parameters. The vertical velocity fluctuation variance throughout the boundary layer can be modeled as

$$\overline{w'^2} = u_*^2 \, f\left(\frac{z}{z_i}, \frac{z}{L}\right)$$

where u_* is the surface friction velocity and L is the Monin-Obhukhov length. These parameters are derivable from the four standard quantities via the use of surface layer profile assumptions. The vertical turbulence scale has also been studied experimentally and theoretically, and can be represented as being proportional to height in the surface layer, reaching a maximum within a mixed layer, and limited by the buoyancy forces under stable stratification. If the profiles of the mean velocity and velocity variance are specified, then the dispersion relations can be used to determine spread rates.

A reasonable estimate for the vertical velocity variance under general conditions is given by

$$\overline{w'^2} = \begin{cases} 1.4u_*^2\left(1-\dfrac{z}{1.3z_i}\right)+u_*^2\left(1.3-\dfrac{z}{z_i}\right)^2\left(\dfrac{z}{k|L|}\right)^{2/3}, & L<0, \quad z<1.3z_i \\ 1.4u_*^2\left(1-\dfrac{z}{5L}\right), & L>0, \quad z<5L \end{cases}$$

indicating the dependence on the generation mechanisms of shear and buoyancy production, and providing the limited vertical extent of the boundary layer mixing. Turbulence intensities can be assumed zero above the limiting heights in the formula.

The situation for surface layer dispersion is somewhat simplified, since the dependence on zi disappears, and the vertical velocity variance can be written entirely in terms of surface layer variables

$$\overline{w'^2} = \begin{cases} u_*^2\left[1.7\left(\dfrac{z}{k|L|}\right)^{2/3}+1.4\right], & L<0 \\ 1.4u_*^2, & L>0\,. \end{cases}$$

The horizontal velocity variance is more complex, in general, since the larger scale horizontal eddies are dependent on parameters outside the surface layer. A simple representation of the horizontal variance for unstable conditions is given by

$$\overline{v'^2} = 2.0u_*^2 + 0.4\left(\frac{z_i}{k|L|}\right)^{2/3}.$$

Horizontal dispersion rates do not scale with surface layer parameters, since the variance cannot be reduced to such a dependence, but the instantaneous horizontal spread rate is probably close to the vertical rate and therefore will exhibit surface layer scaling. The reason for this is that the component energies at the same length scales horizontally and vertically are very similar (i.e., the increased horizontal energy is in larger, meandering scales). However, for longer time averages, the spreads can be very different.

The preceding discussion provides some reason to believe that the PGT predictions should be appropriate for the instantaneous vertical dispersion of a near-surface release. In this case the effects of time-averaging are not significant, since the turbulence timescale is the same as the plume timescales, and furthermore, the turbulence structure is described completely by the wind speed and stability (except for the dependence on surface roughness). We should therefore seek to define the turbulence parameters associated with the PGT stability classes so that the predicted spread using the turbulence relations matches the PGT curves (i.e., we can select a value of L for each stability category to match the PGT spread rate). We do not expect to do this for the horizontal spread, for which the PGT prediction is usually claimed to be representative of a 15 minute average, but is actually dependent on mixed layer depth and other external parameters. Application of this procedure would allow a rational specification of L for each PGT class, but provide a general description of the boundary layer turbulence and its dispersion properties. The improved model should match the vertical dispersion to PGT for short range surface releases and give a more valid description of horizontal dispersion, elevated releases, and longer range effects.

The horizontal turbulence energy depends on z_i, even in the surface layer, so the improved model would give a rational description of the dispersion. The mixed layer depth needs to be specified in addition to the stability category, so a range of values should be tested if a measurement is not available. The additional information provided by specification of the turbulence scales will allow a proper treatment of instantaneous and time averaging effects. In addition, a model based on the use of measurable turbulence quantities will be able to accept site-specific input data.

For the application of the model, we require a value of roughness length, so a typical value for a grass-covered surface, 3 cm, is used. A standard inversion depth, z_i, of 1 km is also specified for the numerical calculations below.

Atmospheric Profiles

The turbulence profiles are described above, but are repeated here for completeness.

(a) Unstable conditions:

$$\overline{w'^2} = w_1^2 + w_2^2 ,$$

$$w_1^2 = 1.4u_*^2\left(1 - \frac{z}{1.3z_i}\right) ,$$

$$w_2^2 = u_*^2\left(1.3 - \frac{z}{z_i}\right)^2 \left(\frac{z}{k|L|}\right)^{2/3} ,$$

$$\overline{v'^2} = v_1^2 + v_2^2 ,$$

$$v_1^2 = 2.0u_*^2\left(1 - \frac{z}{1.3z_i}\right) ,$$

$$v_2^2 = 0.4\left(\frac{z_i}{k|L|}\right)^{2/3} ,$$

$$q^2 = 4w_1^2 + 2w_2^2 .$$

The mean velocity profile can be represented as follows:

$$\overline{u} = \frac{u_*}{k}\left[\ln\left(1 + \frac{z}{z_0}\right) - \psi\right] ,$$

$$\psi = 2 \ln\left(\frac{1 + \phi^{-1}}{2}\right) + \ln\left(\frac{1 + \phi^{-2}}{2}\right) - 2 \tan^{-1}(\phi^{-1}) + \frac{\pi}{2} ,$$

$$\phi = \left(1 - 15 \frac{z}{L}\right)^{-1/4} .$$

for $z \leq 0.5 z_i$. Assume $\bar{u}$ is constant above 0.5 z_i.

The turbulence length scales (as used in the dispersion model below) are:

$$\Lambda_z = \text{MIN}\ (0.65\ z,\ 0.25\ z_i) ,$$
$$\Lambda_y = 0.25\ z_i .$$

where Λ_z is the vertical scale and Λ_y is the horizontal scale.

(b) Stable conditions:

$$\overline{w'^2} = w_1^2 + w_2^2 ,$$

$$w_1^2 = 1.4 u_*^2 \left(1 - \frac{z}{5L}\right) ,$$

$$w_2^2 = 0 ,$$

$$\overline{v'^2} = v_1^2 + v_2^2 ,$$

$$v_1^2 = 2.0\ u_*^2 \left(1 - \frac{z}{5L}\right),$$

$v_2^2 = 0$, unless provided by observations,

$$q^2 = 4 w_1^2 .$$

The mean velocity profile can be represented as follows:

$$\bar{u} = \frac{u_*}{k}\left[\ln\left(1 + \frac{z}{z_0}\right) - \psi\right] ,$$

$$\psi = 4.7\ \frac{z}{L} .$$

for $z < 5L$; $\bar{u}$ is constant above this height.

The vertical turbulence length scale is

$$\Lambda_z = \text{MIN } (0.65\ z,\ 0.2\ L) .$$

Under stable conditions the large scale horizontal turbulence is determined by external conditions (e.g., local terrain), and should therefore be supplied from observations. For instantaneous plume predictions, the vertical turbulence fluctuations can be used.

Dispersion Model

$$\bar{u}\ \frac{d\sigma_z}{dx} = \frac{\sigma_w}{\left[1 + (A_1\sigma_z/\Lambda_w)^2\right]^{1/2}} ,$$

$$\bar{u}\ \frac{d\sigma_z}{dx} = \frac{\sigma_v}{\left[1 + (A_1\sigma_y/\Lambda_v)^2\right]^{1/2}} ,$$

$$\hat{z} = MAX\ (\sigma_z,\ \bar{z}) ,$$

$$A_1 = \frac{Aq}{\sigma_w} .$$

where $\overline{z}$ is the plume centroid, A = 0.75 is a turbulence model constant (Lewellen, 1977). The turbulence parameters used in the dispersion prediction are defined as follows:

$$\sigma_v = \left(\sigma_{v_1}^2 + \sigma_{v_2}^2\right)^{1/2} ,$$

$$\sigma_{v_1}^2 = v_1^2 \left(\frac{\sigma_{T_1}}{\Lambda_y}\right)^{2/3} ,$$

$$\sigma_{v_2}^2 = v_2^2 \left(\frac{\sigma_{T_2}}{\Lambda_z}\right) ,$$

$$\sigma_w^2 = \overline{w'^2} \left(\frac{\sigma_{T_2}}{\Lambda_z}\right) ,$$

$$\sigma_{T_1} = MIN\ (\sigma_T,\ \Lambda_y) ,$$

$$\sigma_{T_2} = MIN\ (\sigma_T,\ \Lambda_z) ,$$

$$\sigma_T = MAX\ (\sigma_y,\ \alpha_u \overline{UT}) ,$$

$$\Lambda_v = \frac{\sigma_{T1}\sigma_{v1}^2 + \sigma_{T_2}\sigma_{V_2}^2}{\sigma_v^2} .$$

where T is the desired averaging time, U is the mean wind speed, and α_u is an empirical constant which is taken to be 0.02 in the calculations below.

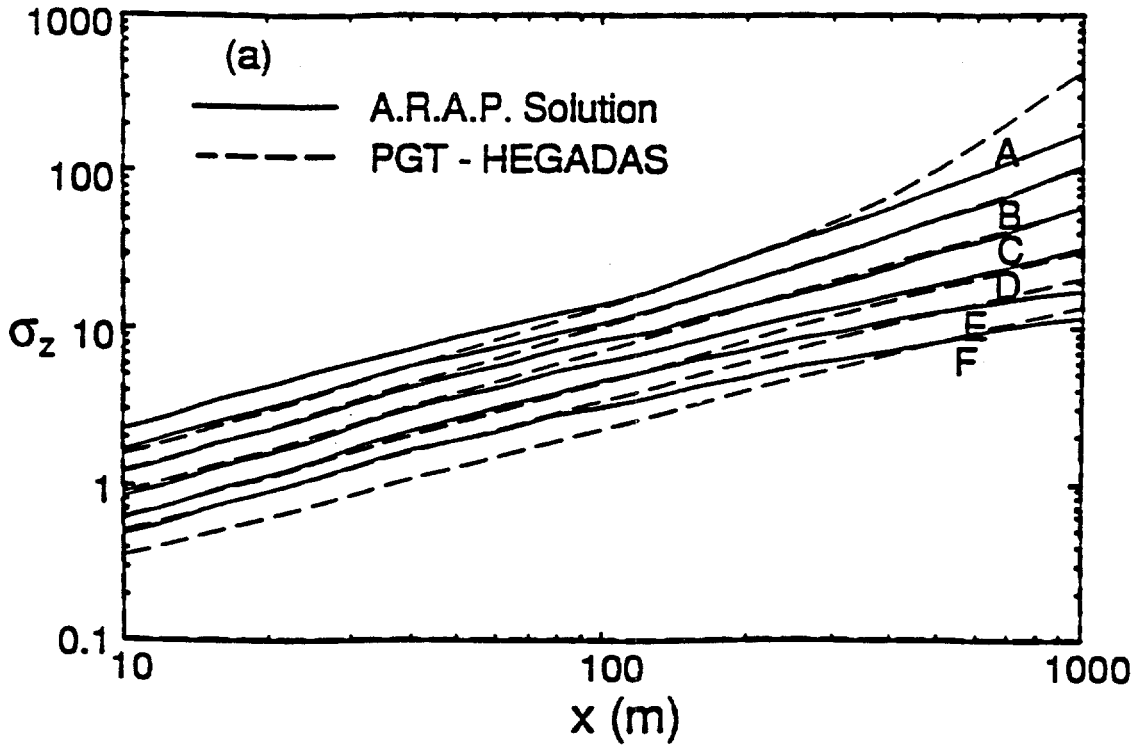
Example Results

The equations introduced above have been solved numerically for a range of input parameters and compared with the PGT-schemes from HEGADAS and PLM89A. Where necessary, a roughness length, z_0, of 3 cm was used and an inversion depth, z_i, of 1000 m. A time average of 900 s was used to compare with the PGT horizontal spread estimates but the vertical spread is effectively independent of the averaging period. The mean wind speed was fixed at 5 ms^{-1}, but this does not influence the vertical spread rate either. An initial source height of 10 m was assumed and the initial source size was effectively zero.

Figure A1 compares the vertical spread predictions with the PGT schemes, and show reasonable agreement over the range of the calculation. The values of L chosen to match the empirical curves are as follows:

Stability A - L = -5 m
Stability B - L = -2.5 m
Stability C - L = -50 m
Stability D - L = ∞
Stability E - L = 25 m
Stability F - L = 13 m

Figure A2 shows the predictions for the horizontal dispersion with an averaging time of 900 s. Stable conditions are not calculated, since the horizontal turbulence is not easily specified in terms of local boundary layer parameters but should be determined from on-site data. The influence of slight instability is evident in the D-category result, where a value of L = -1000 m produces much larger growth at 1 km downstream in comparison with the perfectly neutral case.



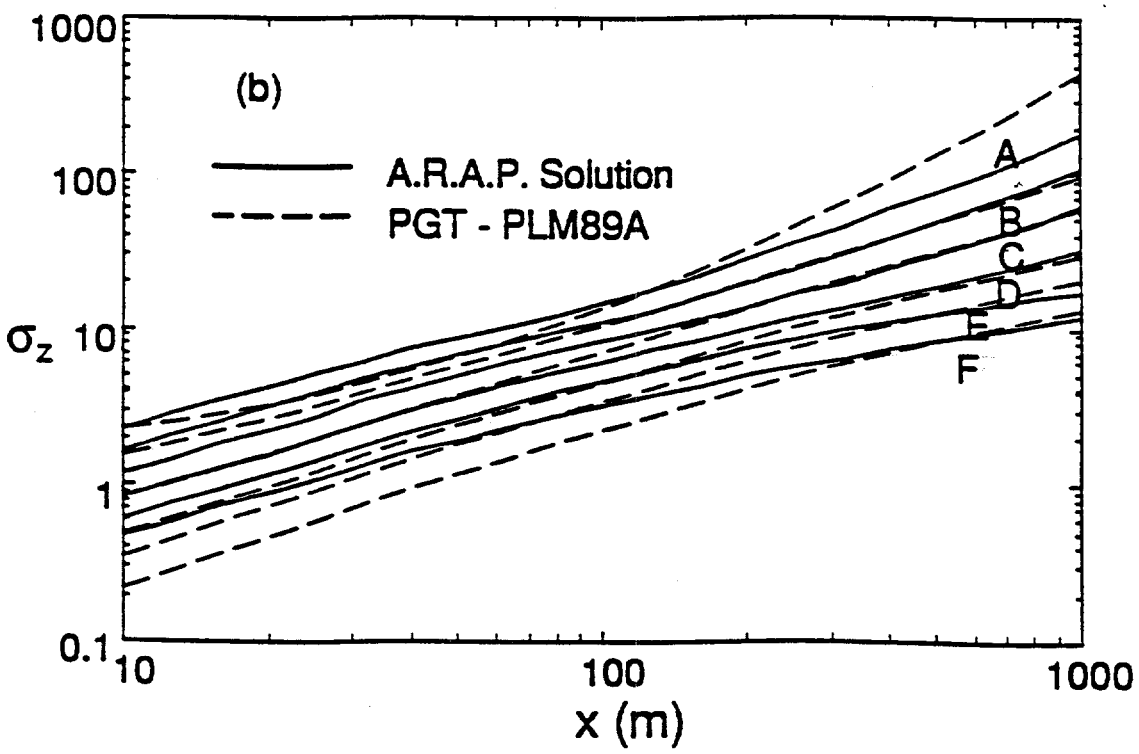


Fig. A.1. Comparison between proposed A.R.A.P. dispersion prediction and PGT scheme from (a) HEGADAS, (b) PLM89A.

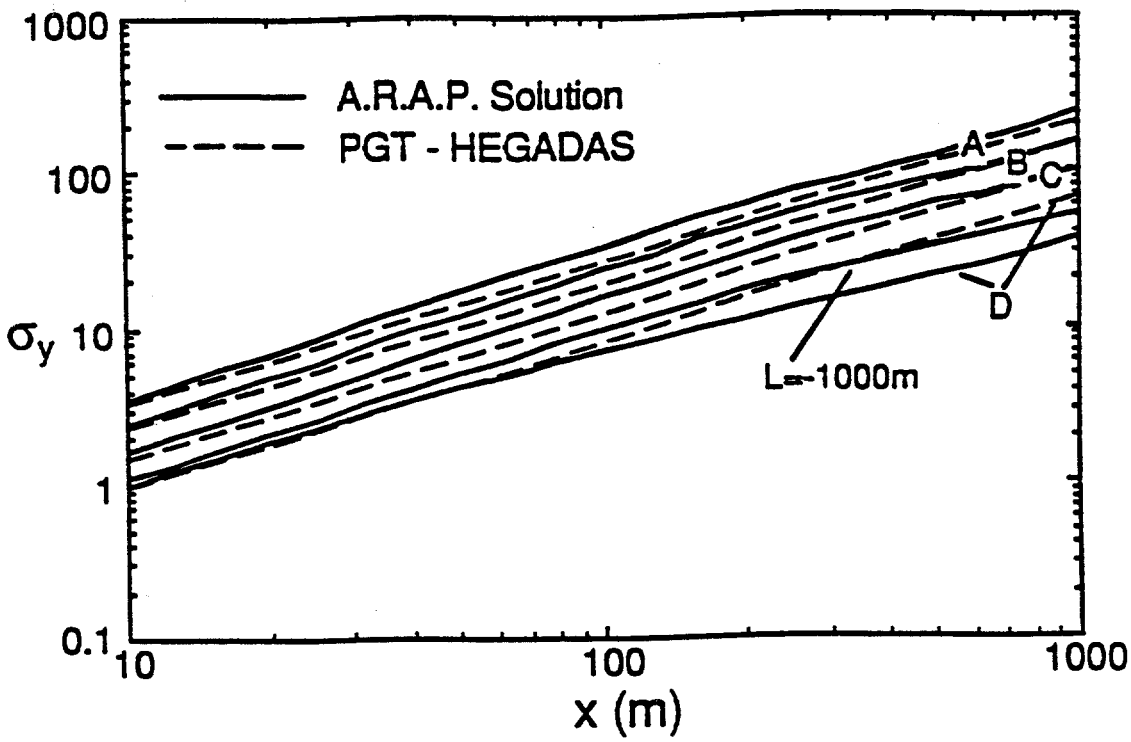


Fig. A2. Comparison between A.R.A.P. dispersion prediction and HEGADAS PGT-scheme for horizontal spread.